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FORTRAN PROGRAM FOR COMPUTING THE PRINCIPAL MOMENTS OF INERTIA OF A RIGID MOLECULE

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SUMMARY

A program to compute the principal moments of inertia of a rigid molecule was written in the FORTRAN language. This program eliminates considerations of symmetry and avoids hand calculations by reducing the input to structural parameters, that is, bond lengths and angles. The assignment of the structural parameters follows geometric models. In its present form the program is written for molecules with not more than 24 atoms.

INTRODUCTION

Many structurally complicated molecular species are becoming of interest at shock-tube and rocket-combustion temperatures. These include polyatomic species, such as HBO_2 and BFCl, which have no axes of symmetry, and polymers, such as $(NaOH)_2$ and $(HBO_2)_3$. Obtaining thermodynamic functions for these species requires that the principal moments of inertia or the product of the principal moments be known. The calculation, however, becomes cumbersome for large molecules or for molecules in which the center of mass and the directions of the principal axes through the center of mass are not immediately apparent. In order to eliminate considerations of symmetry and to avoid hand calculations, the method of reference 1 together with the authors' technique to minimize the input was programed in the FORTRAN language.

The program described herein was used to compute the moments of inertia reported in reference 2. In its present form the program is written for molecules with not more than 24 atoms; however, extension to consider molecules with more than 24 atoms could be easily accomplished. Any set of atomic weights with the corresponding value of Avogadro's number may be selected as input to the program.

The program decks are available from the authors upon request in either FORTRAN II or FORTRAN IV. Also included for the user's convenience are data cards for the atomic weights based on the chemical scale of natural oxygen (O = 16.0000) and the 1961 Table of Atomic Weights (see ref. 3) based on the exact weight of 12 for carbon 12.

SYMBOLS

A	symmetric matrix
I_{xx}, I_{yy}, I_{zz}	moments of inertia
$I_{xy}, I_{yz}, I_{xz}, I_{yx}, I_{zy}, I_{zx}$	products of inertia
M	$\sum_i m_i$
m_i	mass of the i^{th} atom
r	bond length
$r_{i,k}$	bond length between the i^{th} and k^{th} atoms
X,Y	atoms in pyramidal or tetrahedral molecules
x_i, y_i, z_i	Cartesian coordinates of the i^{th} atom
α	angle
θ_i	branch angle with vertex at the i^{th} atom
λ	eigenvalue
σ_i	out-of-plane-atom angle with vertex at the i^{th} atom
φ_i, φ_k	chain angles with vertex at the i^{th} and k^{th} atoms

METHOD OF CALCULATION

The principal moments of inertia are the eigenvalues of the real symmetric matrix A

$$A = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix}$$

The diagonal elements are the moments of inertia about the center of mass; the off-diagonal elements are the products of inertia about the center of mass.

The matrix elements are calculated according to the equations given in reference 1. These equations, where m_i is the mass of the i^{th} atom, x_i, y_i, z_i

are the Cartesian coordinates of this atom, and $M = \sum_i m_i$, are reproduced for convenience:

$$I_{xx} = \sum_i m_i\left(y_i^2 + z_i^2\right) - \frac{1}{M}\left(\sum_i m_i y_i\right)^2 - \frac{1}{M}\left(\sum_i m_i z_i\right)^2$$

$$I_{yy} = \sum_i m_i\left(x_i^2 + z_i^2\right) - \frac{1}{M}\left(\sum_i m_i x_i\right)^2 - \frac{1}{M}\left(\sum_i m_i z_i\right)^2$$

$$I_{zz} = \sum_i m_i\left(x_i^2 + y_i^2\right) - \frac{1}{M}\left(\sum_i m_i x_i\right)^2 - \frac{1}{M}\left(\sum_i m_i y_i\right)^2$$

$$I_{xy} = I_{yx} = -\sum_i m_i x_i y_i + \frac{1}{M}\left(\sum_i m_i x_i\right)\left(\sum_i m_i y_i\right)$$

$$I_{xz} = I_{zx} = -\sum_i m_i x_i z_i + \frac{1}{M}\left(\sum_i m_i x_i\right)\left(\sum_i m_i z_i\right)$$

$$I_{yz} = I_{zy} = -\sum_i m_i y_i z_i + \frac{1}{M}\left(\sum_i m_i y_i\right)\left(\sum_i m_i z_i\right)$$

Any convenient set of orthogonal axes may be chosen to describe a molecule. The equations for the matrix elements give the moments of inertia and the products of inertia about a set of axes parallel to the assigned axes and with origin at the center of mass.

A convenient value in the calculation of thermodynamic properties is the product of the principal moments of inertia. This value is simply the determinant of the matrix A.

The three principal moments of inertia can be found individually as the roots λ of the secular equation

$$\begin{vmatrix} I_{xx} - \lambda & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} - \lambda & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} - \lambda \end{vmatrix} = 0$$

The derivation of this equation is discussed in texts on classical mechanics, such as reference 4.

An attempt to solve directly for the roots of the preceding cubic equation resulted in the appearance of false imaginary solutions, which were caused by inherent machine inaccuracies and rounding errors. Of several other possible methods, the iterative Jacobi method described in reference 5 was chosen to determine the principal moments inasmuch as this method does not depend on the existence of three unequal real roots. In the solution is found an orthogonal matrix, that is, an eigenvector matrix, which transforms the original symmetric matrix A into a diagonal matrix. This is accomplished through the annihilation of selected off-diagonal elements by elementary orthogonal transformations. The elements of the resulting diagonal matrix are the principal moments of inertia.

Because of rounding errors in the computation, the principal moments of inertia are accurate to approximately six significant figures. This degree of accuracy was determined by repeating computations for a molecule after a change in its orientation relative to the assigned axes. This accuracy, however, is adequate in the light of the reliability of experimental structural parameter data.

DISCUSSION OF THE PROGRAM FOR VARIOUS TYPES OF MOLECULES

Figure 1 is a flow diagram of the main program. The block numbers correspond to the statement numbers of the code listing. A flow diagram of the subroutine Jacobi is given in reference 5. The computation of the principal moments of inertia is simplified by equations for the Cartesian coordinates of atoms in terms of the appropriate bond lengths and angles. A molecule is classified according to its geometric type: planar, pyramidal, tetrahedral, other nonplanar, or general. The input for each geometric type follows a specified model. Although this input is reduced to bond lengths and angles, their order of assignment is thus not completely arbitrary.

Each of the six geometric types is illustrated in figure 2 with the equations for the atom coordinates given in table I. Sample computations for each type of input are given in table II. These computations can be used to check the program deck.

Table III is a listing of the code preceded by an explanation of the input cards, and followed by a listing of the input cards used for the computations in table II. The atomic weights and the corresponding Avogadro's number are based on the chemical scale of natural oxygen.

Type 1 - Planar

The input for planar molecules can be reduced to bond lengths and angles when the molecule is considered to be a chain of atoms with other atoms branching from the chain. Planar molecules without and with branching are illustrated in figures 2(a-1) and (a-2), respectively. Figure 2(a-1) represents a molecule such as HBO_2, which has a chain of four atoms; figure 2(a-2) represents a molecule such as $(HBO_2)_3$, which can be visualized as a chain of six atoms with three two-atom branches attached to the chain. The branch atoms are specified according to the chain atom from which they branch, that is, atom 10 is the first

branch atom attached to chain atom 1, and atom 30 is the first branch atom attached to chain atom 3.

The Cartesian coordinates of the atoms are computed by the program from the equations in table I(a). Atom 1 is considered to be at the origin of a set of orthogonal axes and bond $r_{2,3}$ to be parallel to the x-axis. The general equations given in table I(a) will permit the extension of the program to accommodate more chain and branch atoms. Presently, the program can treat a nine-atom chain with two-atom branches from any of the first eight chain atoms.

The necessary input data are the appropriate bond lengths and angles according to the following assignment:

(1) The adjacent bond lengths are specified in order along the chain starting from atom 1 with bond $r_{1,2}$.

(2) The chain angles are specified in order along the chain beginning with angle φ_2 between the first and second bonds. The assigned angles are always on the same side, that is, the "inside," of the chain.

(3) For any particular branch, the bond lengths and branch angles are specified in order from the chain; all angles are taken on the same side of the branch, as indicated in figure 2(a-2).

Although $(HBO_2)_3$ is a closed cyclic structure, it is illustrated in figure 2(a-2) as an open chain with the bond length $r_{6,1}$ and angle φ_6 omitted. These parameters are unnecessary because the preceding bond lengths and angles have specified all the atom positions.

Other chain assignments are also possible for $(HBO_2)_3$, for example, an eight-atom chain with origin at the illustrated atom 11; the two branches would then be attached to the fifth and seventh chain atoms.

The equations for the atom coordinates do not permit branching from the last chain atom. If this error is made in the branch assignment, the computation stops and a suggested assignment is printed.

The input for the simplest chain, a diatomic molecule, consists only of the bond length.

Sample computations for planar molecules without and with branching are given in table II(a).

Type 2 - Pyramidal XY_3

Several molecules such as NH_3, PH_3, PCl_3, and PF_3 are of the pyramidal XY_3 geometric type. The input for this type can be simplified to the X-Y bond length and the Y-X-Y angle.

A three-dimensional pyramidal molecule, oriented relative to a convenient set of orthogonal axes, is illustrated in figure 2(b). The figure also includes diagrams of the atom projections on the xy-, xz-, and yz-planes. The X atom is at the origin of the orthogonal axes and the Y_1 and the Y_2 atoms lie in the xz-plane. The z-axis bisects the Y_1-X-Y_2 angle.

The equations for the Cartesian coordinates of the atoms illustrated in figure 2(b) are given in table I(b). Because of the selection of the coordinate system, these equations are simple functions of the X-Y bond length r and the Y-X-Y angle α.

A sample computation for a pyramidal XY_3 molecule is given in table II(b).

Type 3 - Tetrahedral XY_4

Molecules such as CCl_4, $SiCl_4$, SiF_4, and SiH_4 are of the tetrahedral XY_4 geometric type. The only input necessary for this type is the X-Y bond length.

A three-dimensional tetrahedral molecule, relative to a convenient set of orthogonal axes, is illustrated in figure 2(c). The figure also includes diagrams of the atom projections on the xy-, xz-, and yz-planes. The Y_1, Y_2, and Y_3 atoms lie in the xz-plane with Y_2 on the z-axis, and the X and Y_4 atoms lie on the y-axis.

The equations for the Cartesian coordinates of the atoms illustrated in figure 2(c) are given in table I(c). Because of the selection of the coordinate system, these equations are simple functions of the X-Y bond length r.

Sample computations for the tetrahedral XY_4 molecules are given in table II(c). The input for the P_4 computation involves a fictitious X atom, which is discussed in the section, SPECIAL TREATMENTS OF MOLECULES.

Type 4 - Other Nonplanar

Certain molecules have one or two atoms that are not in the same plane as the other atoms. Examples of these molecules are $(NaOH)_2$, S_2Cl_2, and SF_4. Their out-of-plane atoms are the two H atoms, one Cl atom, and two F atoms, respectively. Three-dimensional diagrams of these molecules, oriented relative to a convenient set of orthogonal axes, are sketched in figure 3. The input is specified by considering the out-of-plane atoms to be special branches from a planar chain. In addition to the bond lengths and angles required for the planar chain input, the out-of-plane-atom (hereinafter called O-P-A) bond length and angle are necessary.

In figure 2(d) a three-dimensional nonplanar molecule is illustrated with the atoms oriented relative to a convenient set of orthogonal axes. The figure also includes diagrams of the atom projections on the xy- and xz-planes. The

out-of-plane atom is specified according to the chain atom from which it branches; that is, out-of-plane atom 200 is attached to chain atom 2. A single-atom O-P-A branch is permitted only from chain atom 2 or 3. This restriction, however, is not severe, and many nonplanar molecules, including all those of interest in reference 2, can be described in this manner.

The Cartesian coordinates of the out-of-plane atoms illustrated in figure 2(d) are computed from the equations in table I(d). The O-P-A bond length $r_{i,k}$ is the distance between the out-of-plane atom and its adjacent chain atom. The O-P-A angle σ_i is formed by the out-of-plane atom, its adjacent chain atom, and one other chain atom, provided that these three atoms form a plane perpendicular to the plane of the chain. The intersection of these two planes is parallel to the x-axis and contains the line segment corresponding to bond length $r_{2,3}$. A plus or a minus sign indicates that the out-of-plane atom is above or below the plane of the chain.

Sample computations for other nonplanar molecules are given in table II(d). Special discussions of the input for the $(NaOH)_2$ and the SF_4 computations are reserved for a later section, SPECIAL TREATMENTS OF MOLECULES.

Types 5 and 6 - General: Coordinates Read In

In these two types the atom coordinates may be read in either in the form $U + V \cos \alpha$ (Type 5) or directly as x,y,z (Type 6). When the orthogonal axes are judiciously chosen, the Cartesian coordinates of the atoms are usually simple functions of the bond lengths and angles. Types 5 and 6 are useful in the computation of principal moments of inertia for molecules not included in the other types and as checks on the other computations.

Examples of Type 5 and Type 6 computations are given in tables II(e) and (f), respectively. The molecules, oriented relative to the assigned coordinate system, are illustrated in figures 2(e) and (f).

SPECIAL TREATMENTS OF MOLECULES

A facility in visualization of structure is helpful in choosing the simplest way of treating a molecule. This is particularly the case with Type 4 - other nonplanar molecules. Occasionally the intuitive order of atoms along a chain is not the most convenient. For instance, the order of the chain atoms for $(NaOH)_2$, illustrated in figure 3(a), was taken to be Na O O in order to accommodate the H atoms as O-P-A branches.

Certain molecules can be made to fit into a desired geometric-type classification by the invention of fictitious atoms of zero mass. The molecule SF_4, shown in figure 3(c), was assigned a fictitious third chain atom in order to permit a planar branch and two O-P-A branches from the second chain atom. Thus the O-P-A plane is perpendicular to the plane of the chain.

Another example of a molecule for which a fictitious atom was invented is P_4. Ordinarily a Type 2 - pyramidal XY_3, this molecule can be treated as a Type 3 - tetrahedral XY_4. In this way, the available experimental data are more easily accommodated. The X atom is fictitious and the four Y atoms correspond to the P atoms. The required bond length input is the fictitious XY bond length, which is readily calculated from the experimental data. Since a fictitious atom has zero mass, it does not affect the principal moments of inertia.

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio, November 13, 1963

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TABLE I. - EQUATIONS FOR THE CARTESIAN COORDINATES OF THE ATOMS

(a) Type 1 - planar

Atom	x-coordinate, angstroms	y-coordinate, angstroms
1	0	0
2	$-r_{1,2} \cos \varphi_2$	$r_{1,2} \sin \varphi_2$
3	$x_2 + r_{2,3}$	y_2
4	$x_3 - r_{3,4} \cos \varphi_3$	$y_3 - r_{3,4} \sin \varphi_3$
5	$x_4 + r_{4,5} \cos(\varphi_3 + \varphi_4)$	$y_4 + r_{4,5} \sin(\varphi_3 + \varphi_4)$
[a] i	$x_{i-1} + (-1)^{i-1} r_{i-1,i} \cos\left(\sum_{k=3}^{i-1} \varphi_k\right)$	$y_{i-1} + (-1)^{i-1} r_{i-1,i} \sin\left(\sum_{k=3}^{i-1} \varphi_k\right)$
10	$-r_{1,10} \cos(\theta_1 - \varphi_2)$	$-r_{1,10} \sin(\theta_1 - \varphi_2)$
11	$x_{10} + r_{10,11} \cos(\theta_1 + \theta_{10} - \varphi_2)$	$y_{10} + r_{10,11} \sin(\theta_1 + \theta_{10} - \varphi_2)$
20	$x_2 + r_{2,20} \cos \theta_2$	$y_2 + r_{2,20} \sin \theta_2$
21	$x_{20} - r_{20,21} \cos(\theta_2 + \theta_{20})$	$y_{20} - r_{20,21} \sin(\theta_2 + \theta_{20})$
30	$x_3 - r_{3,30} \cos(\theta_3 + \varphi_3)$	$y_3 - r_{3,30} \sin(\theta_3 + \varphi_3)$
31	$x_{30} + r_{30,31} \cos(\theta_3 + \theta_{30} + \varphi_3)$	$y_{30} + r_{30,31} \sin(\theta_3 + \theta_{30} + \varphi_3)$
40	$x_4 + r_{4,40} \cos(\theta_4 + \varphi_3 + \varphi_4)$	$y_4 + r_{4,40} \sin(\theta_4 + \varphi_3 + \varphi_4)$
41	$x_{40} - r_{40,41} \cos(\theta_4 + \theta_{40} + \varphi_3 + \varphi_4)$	$y_{40} - r_{40,41} \sin(\theta_4 + \theta_{40} + \varphi_3 + \varphi_4)$
50	$x_5 - r_{5,50} \cos(\theta_5 + \varphi_3 + \varphi_4 + \varphi_5)$	$y_5 - r_{5,50} \sin(\theta_5 + \varphi_3 + \varphi_4 + \varphi_5)$
51	$x_{50} + r_{50,51} \cos(\theta_5 + \theta_{50} + \varphi_3 + \varphi_4 + \varphi_5)$	$y_{50} + r_{50,51} \sin(\theta_5 + \theta_{50} + \varphi_3 + \varphi_4 + \varphi_5)$
[b] 10i	$x_i + (-1)^i r_{i,10i} \cos\left(\theta_i + \sum_{k=3}^{i} \varphi_k\right)$	$y_i + (-1)^i r_{i,10i} \sin\left(\theta_i + \sum_{k=3}^{i} \varphi_k\right)$
[b] 10i+1	$x_{10i} + (-1)^{i-1} r_{10i,10i+1} \cos\left(\theta_i + \theta_{10i} + \sum_{k=3}^{i} \varphi_k\right)$	$y_{10i} + (-1)^{i-1} r_{10i,10i+1} \sin\left(\theta_i + \theta_{10i} + \sum_{k=3}^{i} \varphi_k\right)$

[a] General equations for extension of chain.

[b] General equations for additional branches.

TABLE I. - Concluded. EQUATIONS FOR THE CARTESIAN COORDINATES OF THE ATOMS

(b) Type 2 - pyramidal XY_3

Atom	x-coordinate, angstroms	y-coordinate, angstroms	z-coordinate, angstroms
X	0	0	0
Y_1	$r \sin \frac{\alpha}{2}$	0	$r \cos \frac{\alpha}{2}$
Y_2	$-r \sin \frac{\alpha}{2}$	0	$r \cos \frac{\alpha}{2}$
Y_3	0	$a\left[r^2\left(1 - \frac{k^2}{4 \cos^2 \frac{\alpha}{2}}\right)\right]^{1/2}$	$\frac{rk}{2 \cos \frac{\alpha}{2}}$

(c) Type 3 - tetrahedral XY_4

X	0	r/3	0
Y_1	$r \frac{-\sqrt{6}}{3}$	0	$r \frac{-\sqrt{2}}{3}$
Y_2	0	0	$-2r \frac{-\sqrt{2}}{3}$
Y_3	$-r \frac{-\sqrt{6}}{3}$	0	$r \frac{-\sqrt{2}}{3}$
Y_4	0	$r \frac{4}{3}$	0

(d) Type 4 - other nonplanar

200	$x_2 + r_{2,200} \cos \sigma_2$	y_2	$(\pm) r_{2,200} \sin \sigma_2$
300	$x_3 - r_{3,300} \cos \sigma_3$	y_3	$(\pm) r_{3,300} \sin \sigma_3$

$a_k = 1 - 3 \sin^2 \frac{\alpha}{2} + \cos^2 \frac{\alpha}{2}$.

TABLE II. - SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(a) Type 1

(a-1) HBO_2

PLANAR WITH 4 CHAIN ATOMS AND 0 BRANCHES. WHITE JCP V32 P488 FEB 1960.

NO.	CHAIN ATOM	BOND LENGTH	ANGLE	MOLECULAR WEIGHT	X	Y	Z
1	H			1.00799999	0	0	0
		1.0000					
2	O		120.00	16.0000000	0.49999996	0.86602541	0
		1.3400					
3	B		180.00	10.8199999	1.83999993	0.86602541	0
		1.2000					
4	O			16.0000000	3.03999990	0.86602537	0

THE GENERATED SYMMETRIC MATRIX IS .....

0.1226276	-0.2531333	0
-0.2531333	9.0980780	0
0	0	9.2207053

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 0.11549414
LAMBDA(2)*1.0E+39 = 9.10521126
LAMBDA(3)*1.0E+39 = 9.22070527

PRODUCT LAMBDAS*1.0E+117 = 9.69648027

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

0.11549414	0	0
0	9.10521126	0
0	0	9.22070527

THE EIGENVECTOR MATRIX (S)

0.99960316	-0.28169271E-01	0
0.28169271E-01	0.99960316	0
0	-0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

0.12262755	-0.25313329	0
-0.25313329	9.09807754	0
0	0	9.22070527

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(a) Concluded. Type 1

(a-2) $(HBO_2)_3$

PLANAR WITH 6 CHAIN ATOMS AND 3 BRANCHES. WHITE JCP V32 P488 FEB. 1960 B-O 1.36A, O-H 1.A, CYCLIC

NO.	CHAIN ATOM	BOND LENGTH	ANGLE	MOLECULAR WEIGHT	X	Y	Z
1	B			10.8199999	0	0	0
		1.3600					
2	O		120.00	16.0000000	0.67999993	1.17779455	0
		1.3600					
3	B		120.00	10.8199999	2.03999990	1.17779455	0
		1.3600					
4	O		120.00	16.0000000	2.71999982	-0	0
		1.3600					
5	B		120.00	10.8199999	2.03999972	-1.17779449	0
		1.3600					
6	O			16.0000000	0.67999974	-1.17779440	0

BRANCH NO. 1, ATTACHED TO CHAIN ATOM B , NUMBER 1

NO.	ATOM	BOND LENGTH	ANGLE				
7	O	1.3600	120.00	16.0000000	-1.35999998	-0	0
8	H	1.0000	240.00	1.00799999	-1.86000004	-0.86602537	0

BRANCH NO. 2, ATTACHED TO CHAIN ATOM B , NUMBER 3

NO.	ATOM	BOND LENGTH	ANGLE				
9	O	1.3600	120.00	16.0000000	2.71999997	2.35558903	0
10	H	1.0000	240.00	1.00799999	2.22000015	3.22161448	0

BRANCH NO. 3, ATTACHED TO CHAIN ATOM B , NUMBER 5

NO.	ATOM	BOND LENGTH	ANGLE				
11	O	1.3600	120.00	16.0000000	2.71999946	-2.35558909	0
12	H	1.0000	240.00	1.00799999	3.71999943	-2.35558921	0

THE GENERATED SYMMETRIC MATRIX IS .....

44.624305	-0.3702343E-05	0
-0.3702343E-05	44.624300	0
0	0	89.248606

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 44.6243057
LAMBDA(2)*1.0E+39 = 44.6242971
LAMBDA(3)*1.0E+39 = 89.2486057

PRODUCT LAMBDAS*1.0E+117 = 177723.270

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

44.6243057	0	0
0	44.6242971	0
0	0	89.2486057

THE EIGENVECTOR MATRIX (S)

0.86644093	0.49927959	0
-0.49927959	0.86644093	0
0	0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

44.6243029	-0.35762787E-05	0
-0.40531158E-05	44.6242981	0
0	0	89.2486057

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(b) Type 2 - PCl_3

PYRAMIDAL WITH BOND LENGTH= 2.04300 , AND ANGLE= 100.10
KISLIUK JCP V18 P1109 AUG 1950.

NO.	ATOM	MOLECULAR WEIGHT	X	Y	Z
1	P	30.9749999	0	0	0
2	CL	35.4569998	1.56617413	0	1.31184886
3	CL	35.4569998	-1.56617413	0	1.31184886
4	CL	35.4569998	0	1.96533303	-0.55795603

THE GENERATED SYMMETRIC MATRIX IS .....

32.476808	0	0
0	44.488149	12.625000
0	12.625000	45.746817

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 32.4768076
LAMBDA(2)*1.0E+39 = 32.4768052
LAMBDA(3)*1.0E+39 = 57.7581563

PRODUCT LAMBDAS*1.0E+117 = 60920.0078

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

32.4768076	0	0
0	32.4768052	0
0	0	57.7581563

THE EIGENVECTOR MATRIX (S)

1.00000000	0	0
0	0.72449513	0.68927990
0	-0.68927990	0.72449513

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

32.4768076	0	0
0	44.4881449	12.6249990
0	12.6249990	45.7468128

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(c) Type 3

(c-1) CCl_4

TETRAHEDRAL-REGULAR WITH BOND LENGTH= 1.7600 BARTELL, JCP V23 P1854 OCT 1955.

NO.	ATOM	MOLECULAR WEIGHT	X	Y	Z
1	C	12.0109999	0	0.58666666	0
2	CL	35.4569998	1.43703395	0	0.82967194
3	CL	35.4569998	0	0	-1.65934388
4	CL	35.4569998	-1.43703395	0	0.82967194
5	CL	35.4569998	0	2.34666663	0

THE GENERATED SYMMETRIC MATRIX IS .....

48.625861	0	0
0	48.625861	0
0	0	48.625861

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 48.6258612
LAMBDA(2)*1.0E+39 = 48.6258607
LAMBDA(3)*1.0E+39 = 48.6258612

PRODUCT LAMBDAS*1.0E+117 = 114974.601

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

48.6258612	0	0
0	48.6258607	0
0	0	48.6258612

THE EIGENVECTOR MATRIX (S)

1.00000000	0	0
0	1.00000000	0
0	0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

48.6258612	0	0
0	48.6258607	0
0	0	48.6258612

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(c) Concluded. Type 3

(c-2) P_4

TETRAHEDRAL-REGULAR WITH BOND LENGTH= 1.3533 MAXWELL JCP V3 P699 NOV 1935.

NO.	ATOM	MOLECULAR WEIGHT	X	Y	Z
1		0	0	0.45111433	0
2	P	30.9749999	1.10499991	0	0.63797200
3	P	30.9749999	0	0	-1.27594399
4	P	30.9749999	-1.10499991	0	0.63797200
5	P	30.9749999	0	1.80445731	0

THE GENERATED SYMMETRIC MATRIX IS .....

25.116959	0	0
0	25.116959	0
0	0	25.116960

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 25.1169593
LAMBDA(2)*1.0E+39 = 25.1169593
LAMBDA(3)*1.0E+39 = 25.1169596

PRODUCT LAMBDAS*1.0E+117 = 15845.3263

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

25.1169593	0	0
0	25.1169593	0
0	0	25.1169596

THE EIGENVECTOR MATRIX (S)

1.00000000	0	0
0	1.00000000	0
0	0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

25.1169593	0	0
0	25.1169593	0
0	0	25.1169596

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(d) Type 4

(d-1) $(NaOH)_2$

NON-PLANAR WITH 3 CHAIN ATOMS, 1 PLANAR BRANCHES, AND 2 OUT-OF-PLANE ATOMS.

ESTIMATES FROM NAOH AND LIOH,(LIOH)2.

NO.	CHAIN ATOM	BOND LENGTH	ANGLE	MOLECULAR WEIGHT	X	Y	Z
1	NA			22.9909999	0	0	0
		2.2500					
2	O		40.00	16.0000000	-1.72360000	1.44627209	0
		3.4472					
3	O			16.0000000	1.72359994	1.44627209	0

BRANCH NO. 1, ATTACHED TO CHAIN ATOM O , NUMBER 2

NO.	ATOM	BOND LENGTH	ANGLE				
4	NA	2.2500	40.00	22.9909999	0	2.89254418	0

O-P-A BRANCH NO. 1, ATTACHED TO CHAIN ATOM O , NUMBER 2

NO.	ATOM	BOND LENGTH	O-P-A ANGLE				
5	H	0.9600	120.00	1.00799999	-2.20359993	1.44627209	0.83138438

O-P-A BRANCH NO. 2, ATTACHED TO CHAIN ATOM O , NUMBER 3

NO.	ATOM	BOND LENGTH	O-P-A ANGLE				
6	H	0.9600	120.00	1.00799999	2.20359987	1.44627209	-0.83138438

THE GENERATED SYMMETRIC MATRIX IS .....

16.199666	-0.4701138E-07	0.6131919
-0.4701138E-07	17.639793	-0
0.6131919	-0	33.376763

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 16.1778021
LAMBDA(2)*1.0E+39 = 17.6397927
LAMBDA(3)*1.0E+39 = 33.3986244

PRODUCT LAMBDAS*1.0E+117 = 9531.06799

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

16.1778021	0.72469895E-18	0.55511151E-16
0.72469895E-18	17.6397927	-0.27755576E-16
0.55511151E-16	-0.27755576E-16	33.3986244

THE EIGENVECTOR MATRIX (S)

0.99936502	-0.32111128E-07	0.35630208E-01
0.32135320E-07	0.99999999	-0.10629120E-09
-0.35630208E-01	0.12512118E-08	0.99936503

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

16.1996632	-0.47011378E-07	0.61319189
-0.47011378E-07	17.6397922	0.47184478E-15
0.61319188	-0.16653345E-15	33.3767610

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(d) Continued. Type 4

(d-2) S_2Cl_2

NON-PLANAR WITH 3 CHAIN ATOMS, 0 PLANAR BRANCHES, AND 1 OUT-OF-PLANE ATOMS.

BOWEN, CHEM. SOC., SPECIAL PUBL. NO. 11, 1958.

NO.	CHAIN ATOM	BOND LENGTH	ANGLE	MOLECULAR WEIGHT	X	Y	Z
1	CL			35.4569998	0	0	0
		1.9900					
2	S		104.00	32.0660000	0.48142453	1.93088849	0
		2.0500					
3	S			32.0660000	2.53142446	1.93088849	0

O-P-A BRANCH NO. 1, ATTACHED TO CHAIN ATOM S , NUMBER 3

NO.	ATOM	BOND LENGTH	O-P-A ANGLE				
4	CL	1.9900	104.00	35.4569998	3.01284897	1.93088849	-1.93088849

THE GENERATED SYMMETRIC MATRIX IS .....

32.370342	-17.122919	17.122920
-17.122919	54.089292	5.7624598
17.122920	5.7624598	54.089291

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 14.8526815
LAMBDA(2)*1.0E+39 = 65.8444834
LAMBDA(3)*1.0E+39 = 59.8517456

PRODUCT LAMBDAS*1.0E+117 = 58533.0405

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

14.8526815	0	0.82881942E-12
0	65.8444834	0
0.82881942E-12	0	59.8517456

THE EIGENVECTOR MATRIX (S)

0.81022295	-0.58612171	-0.24990641E-08
0.41445062	0.57291412	0.70710676
-0.41445065	-0.57291416	0.70710672

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

32.3703346	-17.1229138	17.1229153
-17.1229141	54.0892787	5.76245952
17.1229153	5.76245928	54.0892787

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(d) Concluded. Type 4

(d-3) SF_4

NON-PLANAR WITH 3 CHAIN ATOMS, 1 PLANAR BRANCHES, AND 2 OUT-OF-PLANE ATOMS.

DODD TRANS FAR SOC V52 P1052 1956. FICTITIOUS THIRD ATOM.

NO.	CHAIN ATOM	BOND LENGTH	ANGLE	MOLECULAR WEIGHT	X	Y	Z
1	F			19.0000000	0	0	0
		1.5800					
2	S		60.00	32.0660000	-0.79000001	1.36832011	0
		0.7900					
3				0	-0.14901161E-07	1.36832011	0

BRANCH NO. 1, ATTACHED TO CHAIN ATOM S , NUMBER 2

NO.	ATOM	BOND LENGTH	ANGLE				
4	F	1.5800	60.00	19.0000000	0	2.73664021	0

O-P-A BRANCH NO. 1, ATTACHED TO CHAIN ATOM S , NUMBER 2

NO.	ATOM	BOND LENGTH	O-P-A ANGLE				
5	F	1.5800	110.00	19.0000000	-1.33039176	1.36832011	1.48471433

O-P-A BRANCH NO. 2, ATTACHED TO CHAIN ATOM S , NUMBER 2

NO.	ATOM	BOND LENGTH	O-P-A ANGLE				
6	F	1.5800	110.00	19.0000000	-1.33039176	1.36832011	-1.48471433

THE GENERATED SYMMETRIC MATRIX IS .....

25.719417	-0	0
-0	19.548759	-0
0	-0	17.453714

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 25.7194171
LAMBDA(2)*1.0E+39 = 19.5487585
LAMBDA(3)*1.0E+39 = 17.4537139

PRODUCT LAMBDAS*1.0E+117 = 8775.42480

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

25.7194171	-0	0
-0	19.5487585	-0
0	-0	17.4537139

THE EIGENVECTOR MATRIX (S)

1.00000000	0	0
0	1.00000000	0
0	0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

25.7194171	0	0
0	19.5487585	0
0	0	17.4537139

TABLE II. - Continued. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(e) Type 5 - $SOCl_2$

COORDINATES READ IN-- U+VCOS(ALPHA) PALMER JACS V60 P2360 1938. S-O 1.45A, S-CL 2.07A, O-S-CL 106, CL-S-CL 114.

U,V,ALF INPUT

	X			Y			Z		
ATOM	U	V	ALPHA	U	V	ALPHA	U	V	ALPHA
S	-0.	0.	-0.	-0.	-0.	-0.	-0.	-0.	-0.
O	-0.	-0.7338	-0.	-0.	1.2506	-0.	-0.	-0.	-0.
CL	-0.	2.0700	57.0000	-0.	-0.	-0.	-0.	2.0700	33.0000
CL	-0.	2.0700	57.0000	-0.	-0.	-0.	-0.	-2.0700	33.0000

NO.	ATOM	MOLECULAR WEIGHT	X	Y	Z
1	S	32.0660000	0	-0	-0
2	O	16.0000000	-0.73383599	1.25059398	-0
3	CL	35.4569998	1.12740281	-0	1.73604809
4	CL	35.4569998	1.12740281	-0	-1.73604809

THE GENERATED SYMMETRIC MATRIX IS .....

39.079384	4.3422745	-0
4.3422745	45.386801	-0
-0	-0	13.499138

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 36.8664145
LAMBDA(2)*1.0E+39 = 47.5997691
LAMBDA(3)*1.0E+39 = 13.4991376

PRODUCT LAMBDAS*1.0E+117 = 23688.7295

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

36.8664145	0	0
0	47.5997691	0
0	0	13.4991376

THE EIGENVECTOR MATRIX (S)

0.89096754	0.45406698	0
-0.45406698	0.89096754	0
0	0	1.00000000

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

39.0793824	4.34227443	0
4.34227455	45.3867989	0
0	0	13.4991376

TABLE II. - Concluded. SAMPLE COMPUTATION OUTPUTS FOR PRINCIPAL MOMENTS OF INERTIA

(f) Type 6 - S_2Cl_2

COORDINATES READ IN-- X, Y, Z BOWEN, CHEM. SOC., SPECIAL PUBL. NO. 11, 1958.

NO.	ATOM	MOLECULAR WEIGHT	X	Y	Z
1	S	32.0660000	0	0	0
2	S	32.0660000	2.04999998	0	0
3	CL	35.4569998	-0.48142456	1.93088858	0
4	CL	35.4569998	2.53142080	0	1.93088849

THE GENERATED SYMMETRIC MATRIX IS .....

32.370343	17.122910	-17.122889
17.122910	54.089228	5.7624599
-17.122889	5.7624599	54.089231

THE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE PRINCIPAL MOMENTS OF INERTIA (G-SQ CM)

LAMBDA(1)*1.0E+39 = 14.8526877
LAMBDA(2)*1.0E+39 = 65.8444166
LAMBDA(3)*1.0E+39 = 59.8516831

PRODUCT LAMBDAS*1.0E+117 = 58532.9443

THE GENERATED MATRICES FROM THE JACOBI METHOD ARE AS FOLLOWS,

THE DIAGONAL MATRIX (D)

14.8526877	-0.88817842E-15	-0.46649288E-09
-0.88817842E-15	65.8444166	0.45474811E-12
-0.46649288E-09	0.45474811E-12	59.8516831

THE EIGENVECTOR MATRIX (S)

0.81022272	0.58612205	-0.49451341E-06
-0.41445107	0.57291483	0.70710592
0.41445067	-0.57291310	0.70710757

THE MATRIX (S)*(D)*(S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL MATRIX IS,

32.3703361	17.1229050	-17.1228845
17.1229053	54.0892148	5.76245952
-17.1228848	5.76245928	54.0892172

END OF FILE TAPE A 2

TABLE III. - CODE LISTING

```
C MOMENTS OF INERTIA                                                          MOM 001
C PROGRAM COMPUTES PRINCIPAL MOMENTS OF INERTIA FOR THE FOLLOWING TYPE        MOM 002
C  OF SUBSTANCES                                                             MOM 003
C   NTYPE=1   PLANAR                                          EFN 100       MOM 004
C   NTYPE=2   PYRAMIDAL                                       EFN 200       MOM 005
C   NTYPE=3   TETRAHEDRAL                                     EFN 300       MOM 006
C   NTYPE=4   NON-PLANAR WITH OUT-OF-PLANE ATOMS, (O-P-A)     EFN 400       MOM 007
C   NTYPE=5   READ DATA  (U, V, AND ALPHA), FOR EACH X,Y,Z    EFN 500       MOM 008
C   NTYPE=6   READ COORDINATES OF EACH ATOM, X, Y, Z          EFN 600       MOM 009
C                                                                           MOM 010
C                                                                           MOM 011
C                                                                           MOM 012
C PERMANENT INPUT                                                           MOM 013
C                                                                           MOM 014
C CARD 1  CC 1-3   NO. OF ENTRIES IN MOLECULAR WEIGHT TABLES.    INTEGER    MOM 015
C         CC 4-11   EN,  AVOGADRO NO. *1.0E-23                     FLOAT    MOM 016
C         CC 12-19, 20-27, ETC.  MOLECULAR WEIGHTS OF ATOMS,                MOM 017
C                                IN THE ORDER TO BE LISTED ON               MOM 018
C                                NEXT CARD. OVERFLOW ONTO                   MOM 019
C                                ADDITIONAL CARDS IF NECESSARY,             MOM 020
C                                STARTING IN CC1 WITH 8CC/ENTRY,            MOM 021
C                                AND MAXIMUM OF 10 WEIGHTS / CARD.          MOM 022
C CARD 2  NAMES OF ATOMS FOR WHICH MOLECULAR WEIGHTS HAVE BEEN              MOM 023
C   READ IN. 2 CC / NAME, LEFT ADJUSTED, MAXIMUM 40 ATOM NAMES / CARD.      MOM 024
C   OVERFLOW ONTO ADDITIONAL CARDS IF NECESSARY.                            MOM 025
C                                                                           MOM 026
C                                                                           MOM 027
C  INPUT FORMAT FOR EACH SUBSTANCE.                                         MOM 028
C CARD 3  CC 1-78 COMMENTS CARD.                                    ALPH    MOM 029
C         CC 79-80  THE 2 CHARACTERS  C1.                                   MOM 030
C                                                                           MOM 031
C                                                                           MOM 032
C CARD 4  CC 1-3    NUMBER OF ATOMS.                             INTEGER    MOM 033
C         CC 4-6    TYPE OF MOLECULE, NTYPE=1-6 AS LISTED ABOVE. INTEGR    MOM 034
C         CC 7-30   NAME OF SUBSTANCE, EXAMPLE,  BE(OH)2 .         ALPH    MOM 035
C         CC 31-78  NAME OF EACH ATOM, IN DESIRED ORDER,                    MOM 036
C                   2CC/ATOM NAME, LEFT ADJUSTED,                           MOM 037
C                   MAXIMUM 24 ATOMS.  EXAMPLE,  H O BEO H .                MOM 038
C                                                                           MOM 039
C THE REMAINING INPUT DEPENDS ON THE TYPE.                                  MOM 040
C     BOND LENGTHS - ANGSTROMS.                                             MOM 041
C     ANGLES       - DEGREES.                                               MOM 042
C                                                                           MOM 043
C                                                                           MOM 044
CNTYPE=1 ,  PLANAR.                                                         MOM 045
C                                                                           MOM 046
C   CARD 5  CC 1-3  NUMBER OF CHAIN ATOMS = N.                  INTEGER     MOM 047
C           CC 4-6  NUMBER OF BRANCHES   =M.                    INTEGER     MOM 048
C                                                                           MOM 049
C   CARD 6  CC 1-10, 11-20, ETC.,(N-1) BOND LENGTHS,              FLOAT     MOM 050
C                                (N-2) ANGLES,                    FLOAT     MOM 051
C           OVERFLOW ONTO NEXT CARD (6A) IF NECESSARY (MAX 8 WDS./CD)       MOM 052
C           ALL BOND LENGTHS ARE LISTED FIRST, THEN ALL ANGLES.             MOM 053
C                                                                           MOM 054
C     IF THERE ARE ANY PLANAR BRANCHES,                                     MOM 055
C   CARD 7  CC 1-3  NO. OF CHAIN ATOM TO WHICH BRANCH IS ATTACHED.   INT    MOM 056
```

TABLE III. - Continued. CODE LISTING

```
C            CC 4-6  NO. OF ATOMS ON THIS BRANCH  (N).          INTEGER MOM 057
C    CARD 8  CC 1-10, 11-20, ETC., N BOND LENGTHS,  N ANGLES.     FLOAT MOM 058
C                                                                      MOM 059
C      REPEAT CARDS 7 AND 8 FOR EACH PLANAR BRANCH.                    MOM 060
C                                                                      MOM 061
C                                                                      MOM 062
CNTYPE=2 ,  PYRAMIDAL.                                                 MOM 063
C                                                                      MOM 064
C    CARD 5  CC 1-10    BOND LENGTH.                                 FLOAT MOM 065
C            CC 11-20   ANGLE.                                       FLOAT MOM 066
C                                                                      MOM 067
C                                                                      MOM 068
CNTYPE=3 ,  TETRAHEDRAL.                                               MOM 069
C                                                                      MOM 070
C    CARD 5  CC 1-10    BOND LENGTH.                                 FLOAT MOM 071
C                                                                      MOM 072
C                                                                      MOM 073
CNTYPE=4 , NON-PLANAR WITH OUT-OF-PLANE ATOMS, (O-P-A).                MOM 074
C                                                                      MOM 075
C    CARD 5  CC 1-3  NO. OF CHAIN ATOMS.                         INTEGER MOM 076
C            CC 4-6  NO. OF PLANAR BRANCHES.                     INTEGER MOM 077
C            CC 7-9  NO. OF O-P-A BRANCHES.                      INTEGER MOM 078
C                                                                      MOM 079
C    INSTRUCTIONS FOR CARDS 6, 7, AND 8, SAME AS FOR PLANAR, NTYPE=1.  MOM 080
C                                                                      MOM 081
C    CARD 9  CC 1-3  NO. OF CHAIN ATOM  TO WHICH O-P-A BRANCH    INTEGER MOM 082
C                                       IS ATTACHED.                   MOM 083
C            CC 11-20 BOND LENGTH.                                  FLOAT MOM 084
C            CC 21-30 BOND ANGLE.                                   FLOAT MOM 085
C            CC 31-40  SIGN ( +1.0 , OR  -1.0), TO INDICATE ABOVE   FLOAT MOM 086
C                                              OR BELOW THE PLANE.     MOM 087
C      REPEAT CARD 9 FOR EACH O-P-A BRANCH.                            MOM 088
C                                                                      MOM 089
C                                                                      MOM 090
CNTYPE=5 ,  READ DATA (U, V, ALPHA), IN THE FORM U+VCOS(ALPHA),        MOM 091
C                                    FOR X, Y, Z, OF EACH ATOM.        MOM 092
C                                                                      MOM 093
C   CARD5   CC 1- 8   U  , TO CALCULATE  X OF GIVEN ATOM.          FLOAT MOM 094
C           CC 9-16   V  , TO CALCULATE  X OF GIVEN ATOM.          FLOAT MOM 095
C           CC17-24 ALPHA, TO CALCULATE  X OF GIVEN ATOM.          FLOAT MOM 096
C           CC25-32   U  , TO CALCULATE  Y OF GIVEN ATOM.          FLOAT MOM 097
C           CC33-40   V  , TO CALCULATE  Y OF GIVEN ATOM.          FLOAT MOM 098
C           CC41-48 ALPHA, TO CALCULATE  Y OF GIVEN ATOM.          FLOAT MOM 099
C           CC49-56   U  , TO CALCULATE  Z OF GIVEN ATOM.          FLOAT MOM 100
C           CC57-64   V  , TO CALCULATE  Z OF GIVEN ATOM.          FLOAT MOM 101
C           CC65-72 ALPHA, TO CALCULATE  Z OF GIVEN ATOM.          FLOAT MOM 102
C    REPEAT CARD 5 FOR EACH ATOM OF SUBSTANCE, N ATOMS=N CARDS.        MOM 103
C                                                                      MOM 104
C                                                                      MOM 105
CNTYPE=6,  COORDINATES READ IN, X, Y, Z.                               MOM 106
C CARD 5  CC 1-10,11-20,ETC.,   X OF EACH ATOM IN ORDER LISTED.   FLOAT MOM 107
C CARD 6  CC 1-10,11-20,ETC.,   Y OF EACH ATOM IN ORDER LISTED.   FLOAT MOM 108
C CARD 7  CC 1-10,11-20,ETC.,   Z OF EACH ATOM IN ORDER LISTED.   FLOAT MOM 109
      COMMON A,S,SD                                                    MOM 110
      EQUIVALENCE (CHECK,NCHECK),(NCOM,COMENT(14))                     MOM 111
      EQUIVALENCE (A,D)                                                MOM 112
```

TABLE III. - Continued. CODE LISTING

```
      DIMENSION A(3,3),D(3,3),S(3,3),SD(3,3)                                MOM 113
      DIMENSION SUBS(4),COMENT(14),MOL(26),X(26),Y(26),Z(26),EMN(26),EM(MOM 114
     126),WGHT(105),NAME(105),BOND(25),ANG(24),V(3),ANGBR(2)                MOM 115
C                                                                           MOM 116
C SET IT1 = TO NUMBER OF INPUT TAPE                                         MOM 117
C                                                                           MOM 118
C SET IT2 = TO NUMBER OF OUTPUT TAPE                                        MOM 119
C                                                                           MOM 120
      IT1=7                                                                 MOM 121
      IT2=6                                                                 MOM 122
C                                                                           MOM 123
      RAD=0.0174532925                                                      MOM 124
C                                                                           MOM 125
C READ PERMANENT DATA.                                                      MOM 126
C                                                                           MOM 127
      READ INPUT TAPE IT1,1002,NTABL,EN,(WGHT(J),J=1,NTABL)                 MOM 128
      NTABL=NTABL+1                                                         MOM 129
      WGHT(NTABL)=0.                                                        MOM 130
      READ INPUT TAPE IT1,1006,(NAME(J),J=1,NTABL)                          MOM 131
C                                                                           MOM 132
C READ INPUT CARDS 3 AND 4. INPUT FOR EACH SUBSTANCE.                       MOM 133
C                                                                           MOM 134
  900 READ INPUT TAPE IT1,1003,(COMENT(J),J=1,14)                           MOM 135
  901 READ INPUT TAPE IT1,1000,NATMS,NTYPE,(SUBS(J),J=1,4),                 MOM 136
     1(MOL(J),J=1,NATMS)                                                    MOM 137
      WRITE OUTPUT TAPE IT2,2015,(SUBS(J),J=1,4)                            MOM 138
      SWITCH=0.                                                             MOM 139
C                                                                           MOM 140
C GET MOLECULAR WEIGHT OF EACH ATOM                                         MOM 141
C                                                                           MOM 142
      DO 801 J=1,NATMS                                                      MOM 143
      IF(MOL(J)-NAMOLD)802,803,802                                          MOM 144
  803 EMN(J)=WTOLD                                                          MOM 145
      GO TO 40                                                              MOM 146
  802 DO 804 K=1,NTABL                                                      MOM 147
      IF(MOL(J)-NAME(K))804,805,804                                         MOM 148
  805 KK=K                                                                  MOM 149
      GO TO 806                                                             MOM 150
  804 CONTINUE                                                              MOM 151
      GO TO 831                                                             MOM 152
  806 EMN(J)=WGHT(KK)                                                       MOM 153
      NAMOLD=NAME(KK)                                                       MOM 154
      WTOLD=WGHT(KK)                                                        MOM 155
   40 EM(J)=EMN(J)/EN                                                       MOM 156
  801 CONTINUE                                                              MOM 157
C                                                                           MOM 158
C TRANSFER ACCORDING TO NTYPE, TO INPUT REMAINING DATA.                     MOM 159
C                                                                           MOM 160
      GO TO (100,200,300,400,500,600),NTYPE                                 MOM 161
C                                                                           MOM 162
C ERROR WRITE OUT, AND GO ON TO NEXT CASE.                                  MOM 163
C                                                                           MOM 164
  831 CONTINUE                                                              MOM 165
      WRITE OUTPUT TAPE IT2,2016,MOL(J)                                     MOM 166
  810 WRITE OUTPUT TAPE IT2,2020,(SUBS(I),I=1,4)                            MOM 167
B     CHECK=230160606060                                                    MOM 168
```

TABLE III. - Continued. CODE LISTING

```
  825 READ INPUT TAPE IT1,1003,(COMENT(J),J=1,14)                          MOM 169
      DIFC=NCHECK-NCOM                                                     MOM 170
B     IF(DIFC*777777777777)825,901,825                                     MOM 171
C                                                                          MOM 172
C PLANAR SUBSTANCES INPUT                                                  MOM 173
C                                                                          MOM 174
  100 READ INPUT TAPE IT1,1005,NCHAIN,NBRAN                                MOM 175
      WRITE OUTPUT TAPE IT2,2100,NCHAIN,NBRAN,(COMENT(J),J=1,13)           MOM 176
  105 DO 101 J=1,NATMS                                                     MOM 177
  101 Z(J)=0.                                                              MOM 178
      X(1)=0.                                                              MOM 179
      Y(1)=0.                                                              MOM 180
      N=1                                                                  MOM 181
      IF(NCHAIN-2)132,102,102                                              MOM 182
  132 WRITE OUTPUT TAPE IT2,2018,NCHAIN                                    MOM 183
      GO TO 810                                                            MOM 184
  102 NM1=NCHAIN-1                                                         MOM 185
      NM2=NCHAIN-2                                                         MOM 186
      READ INPUT TAPE IT1,1001,(BOND(J),J=1,NM1),(ANG(J),J=1,NM2)          MOM 187
      IF(ANG(1))115,116,115                                                MOM 188
  115 ANGLE=(180.0-ANG(1))*RAD                                             MOM 189
  116 X(2)=(BOND(1))*COSF(ANGLE)                                           MOM 190
      Y(2)=BOND(1)*SINF(ANGLE)                                             MOM 191
      ANGDEG=0.                                                            MOM 192
      DO 112 J=3,NCHAIN                                                    MOM 193
      ANGLE=ANGDEG*RAD                                                     MOM 194
      SIGN=(-1)**(J-1)                                                     MOM 195
      X(J)=X(J-1)+SIGN*BOND(J-1)*COSF(ANGLE)                               MOM 196
      IF(MODF(ANGDEG,180.))114,113,114                                     MOM 197
  113 SIGN=0.                                                              MOM 198
  114 Y(J)=Y(J-1)+SIGN*BOND(J-1)*SINF(ANGLE)                               MOM 199
  112 ANGDEG=ANGDEG+ANG(J-1)                                               MOM 200
      WRITE OUTPUT TAPE IT2,2108,N,MOL(1),EMN(1),X(1),Y(1),Z(1),BOND(1)    MOM 201
      IF(NCHAIN-2)1044,1044,1045                                           MOM 202
 1045 WRITE OUTPUT TAPE IT2,2101,(J,MOL(J),ANG(J-1),EMN(J),X(J),Y(J),      MOM 203
     1Z(J),BOND(J),J=2,NM1)                                                MOM 204
 1044 N=NCHAIN                                                             MOM 205
      WRITE OUTPUT TAPE IT2,2102,N,MOL(N),EMN(N),X(N),Y(N),Z(N)            MOM 206
      N=N+1                                                                MOM 207
  104 IF(NBRAN)103,135,103                                                 MOM 208
  103 CONTINUE                                                             MOM 209
      DO 130 L=1,NBRAN                                                     MOM 210
      READ INPUT TAPE IT1,1005,NATCH,NBRATS                                MOM 211
      IF(NCHAIN-NATCH)107,107,106                                          MOM 212
  107 WRITE OUTPUT TAPE IT2,2021,NCHAIN,NATCH                              MOM 213
      GO TO 810                                                            MOM 214
  106 READ INPUT TAPEIT1,1001,(BOND(J),J=1,NBRATS),(ANGBR(J),J=1,NBRATS)MOM 215
      NP1=N+1                                                              MOM 216
      NN=NATCH                                                             MOM 217
      NNN=1                                                                MOM 218
      M=N                                                                  MOM 219
  128 ASSIGN 127 TO NNNN                                                   MOM 220
      IF(NATCH-2)121,122,123                                               MOM 221
  121 ANGDEG=ANGBR(1)-ANG(1)                                               MOM 222
      GO TO 125                                                            MOM 223
  122 ANGDEG=ANGBR(1)                                                      MOM 224
```

TABLE III. - Continued. CODE LISTING

```
      GO TO 125                                                          MOM 225
  123 ANGDEG=ANGBR(1)                                                    MOM 226
      NAM1=NATCH-1                                                       MOM 227
      DO 124 J=2,NAM1                                                    MOM 228
  124 ANGDEG=ANGDEG+ANG(J)                                               MOM 229
  125 SIGN=(-1.0)**NATCH                                                 MOM 230
  129 ANGLE=ANGDEG*RAD                                                   MOM 231
      X(M)=X(NN)+SIGN*BOND(NNN)*COSF(ANGLE)                              MOM 232
      Y(M)=Y(NN)+SIGN*BOND(NNN)*SINF(ANGLE)                              MOM 233
      IF(NBRATS-1)145,134,136                                            MOM 234
  136 GO TO NNNN,(127,134)                                               MOM 235
  127 ANGDEG=ANGDEG+ANGBR(2)                                             MOM 236
      SIGN=-SIGN                                                         MOM 237
      NN=N                                                               MOM 238
      NNN=2                                                              MOM 239
      M=M+1                                                              MOM 240
      ASSIGN 134 TO NNNN                                                 MOM 241
      GO TO 129                                                          MOM 242
  134 WRITE OUTPUT TAPE IT2,2103,L,MOL(NATCH),NATCH                      MOM 243
      DO 131 KK=1,NBRATS                                                 MOM 244
      NN=N-1+KK                                                          MOM 245
  131 WRITE OUTPUT TAPE IT2,2104,NN,MOL(NN),BOND(KK),ANGBR(KK),EMN(NN),  MOM 246
     1X(NN),Y(NN),Z(NN)                                                  MOM 247
  130 N=N+NBRATS                                                         MOM 248
  135 IF(SWITCH(1)401,800,401                                            MOM 249
  145 WRITE OUTPUT TAPE IT2,2125,NBRATS,L,MOL(NATCH),NATCH,MOL(N),       MOM 250
     1MOL(NP1)                                                           MOM 251
      GO TO 810                                                          MOM 252
C                                                                        MOM 253
C   INPUT FOR PYRAMIDAL       XY3       ALWAYS 4 ATOMS-- X, Y, Y, Y    MOM 254
C   BLN=X-Y BOND LENGTH,  ALF= Y-X-Y ANGLE                               MOM 255
C                                                                        MOM 256
  200 CONTINUE                                                           MOM 257
      READ INPUT TAPE IT1,1001,BLN,ALF                                   MOM 258
      WRITE OUTPUT TAPE IT2,2106,BLN,ALF,(COMENT(J),J=1,13)              MOM 259
      ANGL=(ALF/2.)*RAD                                                  MOM 260
      SINAL=SINF(ANGL)                                                   MOM 261
      COSAL=COSF(ANGL)                                                   MOM 262
      SISQ=SINAL**2                                                      MOM 263
      COSQ=COSAL**2                                                      MOM 264
      X(1)=0.                                                            MOM 265
      X(2)=BLN*SINAL                                                     MOM 266
      X(3)=-X(2)                                                         MOM 267
      X(4)=0.                                                            MOM 268
      Y(1)=0.                                                            MOM 269
      Y(2)=0.                                                            MOM 270
      Y(3)=0.                                                            MOM 271
      TEM=(1.-3.*SISQ+COSQ)/(2.*COSAL)                                   MOM 272
      Y(4)=SQRTF(BLN**2*(1.-TEM**2))                                     MOM 273
      Z(1)=0.                                                            MOM 274
      Z(2)=BLN*COSAL                                                     MOM 275
      Z(3)=Z(2)                                                          MOM 276
      Z(4)=BLN*TEM                                                       MOM 277
      GO TO 815                                                          MOM 278
C                                                                        MOM 279
C   INPUT FOR TETRAHEDRAL-REGULAR  XY4 ALWAYS 5 ATOMS---X Y Y Y Y       MOM 280
```

TABLE III. - Continued. CODE LISTING

```
C  BLN=X-Y BOND LENGTH                                                    MOM 281
C                                                                         MOM 282
  300 CONTINUE                                                            MOM 283
      READ INPUT TAPE IT1,1001,BLN                                        MOM 284
      WRITE OUTPUT TAPE IT2,2105,BLN,(COMENT(J),J=1,13)                   MOM 285
      X(1)=0.                                                             MOM 286
      X(2)=BLN*0.81649658                                                 MOM 287
      X(3)=0.                                                             MOM 288
      X(4)=-X(2)                                                          MOM 289
      X(5)=0.                                                             MOM 290
      Y(1)=BLN/3.                                                         MOM 291
      Y(2)=0.                                                             MOM 292
      Y(3)=0.                                                             MOM 293
      Y(4)=0.                                                             MOM 294
      Y(5)=BLN*1.33333333                                                 MOM 295
      Z(1)=0.                                                             MOM 296
      Z(2)=BLN*0.47140452                                                 MOM 297
      Z(3)=-2.*Z(2)                                                       MOM 298
      Z(4)=Z(2)                                                           MOM 299
      Z(5)=0.                                                             MOM 300
      GO TO 815                                                           MOM 301
C                                                                         MOM 302
C NON-PLANAR WITH OUT OF PLANE ATOMS                                      MOM 303
C                                                                         MOM 304
  400 CONTINUE                                                            MOM 305
      READ INPUT TAPE IT1,1005,NCHAIN,NBRAN,NOPA                          MOM 306
      WRITE OUTPUT TAPE IT2,2400,NCHAIN,NBRAN,NOPA,(COMENT(J),J=1,13)     MOM 307
      SWITCH=0.1                                                          MOM 308
      GO TO 105                                                           MOM 309
  401 DO 410 L=1,NOPA                                                     MOM 310
      READ INPUT TAPE IT1,1007,NATCH,BLN,ANGDEG,SIGNOP                    MOM 311
      ANGLE=ANGDEG*RAD                                                    MOM 312
      GO TO (402,402,403),NATCH                                           MOM 313
  402 SIGN=+1.0                                                           MOM 314
      GO TO 405                                                           MOM 315
  403 SIGN=-1.0                                                           MOM 316
  405 X(N)=X(NATCH)+SIGN*BLN*COSF(ANGLE)                                  MOM 317
      Y(N)=Y(NATCH)                                                       MOM 318
      Z(N)=SIGNOP*BLN*SINF(ANGLE)                                         MOM 319
  404 WRITE OUTPUT TAPE IT2,2401,L,MOL(NATCH),NATCH                       MOM 320
      WRITE OUTPUT TAPE IT2,2104,N,MOL(N),BLN,ANGDEG,EMN(N),X(N),Y(N),    MOM 321
     1Z(N)                                                                MOM 322
  410 N=N+1                                                               MOM 323
      GO TO 800                                                           MOM 324
C                                                                         MOM 325
C COORDINATES READ IN--U+V*COS(ALPHA)                                     MOM 326
C                                                                         MOM 327
  500 CONTINUE                                                            MOM 328
      WRITE OUTPUT TAPE IT2,2500,(COMENT(J),J=1,13)                       MOM 329
      DO 501 L=1,NATMS                                                    MOM 330
      READ INPUT TAPE IT1,1500,(BOND(J),V(J),ANG(J),J=1,3)                MOM 331
      WRITE OUTPUT TAPE IT2,2501,MOL(L),(BOND(J),V(J),ANG(J),J=1,3)       MOM 332
      X(L)=BOND(1)+V(1)*(COSF(ANG(1)*RAD))                                MOM 333
      Y(L)=BOND(2)+V(2)*(COSF(ANG(2)*RAD))                                MOM 334
      Z(L)=BOND(3)+V(3)*(COSF(ANG(3)*RAD))                                MOM 335
  501 CONTINUE                                                            MOM 336
```

TABLE III. - Continued. CODE LISTING

```
      GO TO 815                                                          MOM 337
C                                                                        MOM 338
C COORDINATES READ IN---X, Y, Z                                          MOM 339
C  SPECIAL FOR MOLECULES NOT CATEGORIZED                                 MOM 340
C                                                                        MOM 341
  600 CONTINUE                                                           MOM 342
      READ INPUT TAPE IT1,1001,(X(J),J=1,NATMS)                          MOM 343
      READ INPUT TAPE IT1,1001,(Y(J),J=1,NATMS)                          MOM 344
      READ INPUT TAPE IT1,1001,(Z(J),J=1,NATMS)                          MOM 345
      WRITE OUTPUT TAPE IT2,2600,(COMENT(J),J=1,13)                      MOM 346
  815 WRITE OUTPUT TAPE IT2,2019,(J,MOL(J),EMN(J),X(J),Y(J),Z(J),        MOM 347
     1J=1,NATMS)                                                         MOM 348
C                                                                        MOM 349
C COMPUTE ELEMENTS OF SYMMETRIC MATRIX, A.                               MOM 350
C                                                                        MOM 351
  800 CONTINUE                                                           MOM 352
      EMM=0.                                                             MOM 353
      SMX=0.                                                             MOM 354
      SMY=0.                                                             MOM 355
      SMZ=0.                                                             MOM 356
      SXY=0.                                                             MOM 357
      SXZ=0.                                                             MOM 358
      SYZ=0.                                                             MOM 359
      SMXY=0.                                                            MOM 360
      SMXZ=0.                                                            MOM 361
      SMYZ=0.                                                            MOM 362
      DO 10 J=1,NATMS                                                    MOM 363
      EMM=EMM+EM(J)                                                      MOM 364
      EMX=EM(J)*X(J)                                                     MOM 365
      EMY=EM(J)*Y(J)                                                     MOM 366
      XSQ=X(J)**2                                                        MOM 367
      YSQ=Y(J)**2                                                        MOM 368
      ZSQ=Z(J)**2                                                        MOM 369
      SMX=SMX+EMX                                                        MOM 370
      SMY=SMY+EMY                                                        MOM 371
      SMZ=SMZ+(EM(J)*Z(J))                                               MOM 372
      SMXY=SMXY+(EMX*Y(J))                                               MOM 373
      SMXZ=SMXZ+(EMX*Z(J))                                               MOM 374
      SMYZ=SMYZ+(EMY*Z(J))                                               MOM 375
      SXY=SXY+(EM(J)*(XSQ+YSQ))                                          MOM 376
      SXZ=SXZ+(EM(J)*(XSQ+ZSQ))                                          MOM 377
      SYZ=SYZ+(EM(J)*(YSQ+ZSQ))                                          MOM 378
   10 CONTINUE                                                           MOM 379
      SMXSQ=SMX**2                                                       MOM 380
      SMYSQ=SMY**2                                                       MOM 381
      SMZSQ=SMZ**2                                                       MOM 382
      EY11=SYZ-((SMYSQ+SMZSQ)/EMM)                                       MOM 383
      EY22=SXZ-((SMXSQ+SMZSQ)/EMM)                                       MOM 384
      EY33=SXY-((SMYSQ+SMXSQ)/EMM)                                       MOM 385
      EY12=SMX*SMY/EMM-SMXY                                              MOM 386
      EY13=SMX*SMZ/EMM-SMXZ                                              MOM 387
      EY23=SMY*SMZ/EMM-SMYZ                                              MOM 388
      A(1,1)=EY11                                                        MOM 389
      A(2,2)=EY22                                                        MOM 390
      A(3,3)=EY33                                                        MOM 391
      A(1,2)=EY12                                                        MOM 392
```

TABLE III. - Continued. CODE LISTING

```
      A(2,1)=EY12                                                       MOM 393
      A(1,3)=EY13                                                       MOM 394
      A(3,1)=EY13                                                       MOM 395
      A(2,3)=EY23                                                       MOM 396
   11 A(3,2)=EY23                                                       MOM 397
C                                                                       MOM 398
C GET EIGENVALUES.                                                      MOM 399
C                                                                       MOM 400
      CALL JACOBI(3,1.0E-9)                                             MOM 401
      PRODD=D(1,1)*D(2,2)*D(3,3)                                        MOM 402
C                                                                       MOM 403
C WRITE OUT MATRICES AND EIGENVALUES.                                   MOM 404
C                                                                       MOM 405
      WRITE OUTPUT TAPE IT2,2200,EY11,EY12,EY13,D(1,1),D(2,2),EY12,EY22,MOM 406
     1EY23,D(3,3),EY13,EY23,EY33,PRODD                                  MOM 407
  820 WRITE OUTPUT TAPE IT2,2201,(((D(I,J),J=1,3),(S(I,J),J=1,3)),I=1,3)MOM 408
      WRITE OUTPUT TAPE IT2,2202,((SD(I,J),J=1,3),I=1,3)                MOM 409
C                                                                       MOM 410
C GO TO READ DATA FOR A NEW CASE.                                       MOM 411
C                                                                       MOM 412
      GO TO 900                                                         MOM 413
 1000 FORMAT(2I3,4A6,25A2)                                              MOM 414
 1001 FORMAT(8F10.4)                                                    MOM 415
 1002 FORMAT(I3,9F8.3/(10F8.3))                                         MOM 416
 1003 FORMAT(13A6,A2)                                                   MOM 417
 1005 FORMAT(3I3)                                                       MOM 418
 1006 FORMAT(40A2)                                                      MOM 419
 1007 FORMAT(I3,7X,3F10.4)                                              MOM 420
 1500 FORMAT(9F8.4)                                                     MOM 421
 2015 FORMAT(1H1,15X,33HPRINCIPAL MOMENTS OF INERTIA OF   4A6)          MOM 422
 2016 FORMAT(13HL THIS ATOM  A6,36HIS NOT IN THE NAME AND WEIGHT TABLE.)MOM 423
 2018 FORMAT(52HL   NO. OF CHAIN ATOMS IS LESS THAN 2.       NCHAIN= I5)MOM 424
 2019 FORMAT(1HK,5X,3HNO.,6X,4HATOM,7X,16HMOLECULAR WEIGHT,6X,1HX,16X,  MOM 425
     11HY,16X,1HZ/(1HJ,I7,8X,A6,4X,4G17.8))                             MOM 426
 2020 FORMAT(30HL   THIS CASE, SUBSTANCE IS   4A6,48H, CANNOT BE CONTINUMOM 427
     1ED, GO ON TO NEXT SUBSTANCE.      )                               MOM 428
 2021 FORMAT(58HL   BRANCH IS ATTACHED TO LAST OR NO CHAIN ATOM. THERE AMOM 429
     1RE I3,54H CHAIN ATOMS, THE BRANCH IS ATTACHED TO CHAIN ATOM NO.I3)MOM 430
 2100 FORMAT(14HK  PLANAR WITH I3,16H CHAIN ATOMS AND I3,10H BRANCHES., MOM 431
     14X, 13A6)                                                         MOM 432
 2101 FORMAT(I8,8X,A6,15X,F9.2,4X,4G17.8/F35.4)                         MOM 433
 2102 FORMAT(I8,8X,A6,28X,4G17.8)                                       MOM 434
 2103 FORMAT(1HK,6X,10HBRANCH NO. I3,26H, ATTACHED TO CHAIN ATOM  A6,    MOM 435
     1 9H,  NUMBER I3/1HJ,5X,3HNO.,6X,4HATOM,7X,11HBOND LENGTH,4X,      MOM 436
     25HANGLE /)                                                        MOM 437
 2104 FORMAT(I8,8X,A6,F13.4,F11.2,4X,4G17.8)                            MOM 438
 2105 FORMAT(40HL  TETRAHEDRAL-REGULAR WITH BOND LENGTH= F8.4 ,3X,      MOM 439
     113A6)                                                             MOM 440
 2106 FORMAT(30HL  PYRAMIDAL WITH BOND LENGTH= F10.5,13H , AND ANGLE=   MOM 441
     1F10.2/40X, 13A6,A2)                                               MOM 442
 2107 FORMAT(1HJ,40X,13A6,A2)                                           MOM 443
 2108 FORMAT(1HK,5X,60HNO.   CHAIN ATOM    BOND LENGTH    ANGLE    MOLECMOM 444
     1ULAR WEIGHT,7X,1HX,16X,1HY,16X,1HZ/1HJ,I7,8X,A6,28X,4G17.8/F35.4) MOM 445
 2125 FORMAT(61HL  NO. OF BRANCH ATOMS IS =, OR LESS THAN 0.  NBRANCH ATMOM 446
     10MS= I4,20H  THIS IS BRANCH NO. I4/26H, ATTACHED TO CHAIN ATOM 6, MOM 447
     29H, NUMBER I4,30H. THE ATOMS ON THIS BRANCH ARE 2A6)              MOM 448
```

TABLE III. - Continued. CODE LISTING

```
2200 FORMAT(44HL   THE GENERATED SYMMETRIC MATRIX IS ......,36X,        MOM 449
    2 46HTHE EIGENVALUES, LAMBDA, OF THE MATRIX ARE THE/80X,            MOM 450
    3 39HPRINCIPAL MOMENTS OF INERTIA  (G-SQ CM)/8X,1HI,55X,1HI/        MOM 451
    4 8X,1HI,3G17.7,4X,1HI/8X,1HI,55X,1HI,18X,19HLAMBDA(1)*1.0E+39 =    MOM 452
    5 G16.8/8X,1HI,55X,1HI,18X,19HLAMBDA(2)*1.0E+39 =G16.8/8X,1HI,      MOM 453
    6 3G17.7,4X,1HI,18X,19HLAMBDA(3)*1.0E+39 =G16.8/8X,1HI,55X,1HI/     MOM 454
    7 8X,1HI,55X,1HI/8X,1HI,3G17.7,4X,1HI,18X,26HPRODUCT LAMBDAS*1.0E+1MOM 455
    817 =G16.8/8X,1HI,55X,1HI)                                          MOM 456
2201 FORMAT(1H1,4X,61HTHE GENERATED MATRICES FROM THE JACOBI METHOD AREMOM 457
    1 AS FOLLOWS,/1HK,4X, 24HTHE DIAGONAL MATRIX (D) ,40X, 27HTHE EIGENMOM 458
    2VECTOR MATRIX (S) / 2HJI,58X,1HI, 9X,1HI,58X,1HI/                  MOM 459
    3          2H I,G16.8,2G20.8,2X,1HI, 9X,1HI,G16.8,2G20.8,2X,1HI/    MOM 460
    4          2H I,58X,1HI,9X,1HI,58X,1HI/                             MOM 461
    5          2H I,G16.8,2G20.8,2X,1HI, 9X,1HI,G16.8,2G20.8,2X,1HI/    MOM 462
    6          2H I,58X,1HI,9X,1HI,58X,1HI/                             MOM 463
    7          2H I,G16.8,2G20.8,2X,1HI, 9X,1HI,G16.8,2G20.8,2X,1HI/    MOM 464
    8          2H I,58X,1HI,9X,1HI,58X,1HI)                             MOM 465
2202 FORMAT(1HL,4X, 39HTHE MATRIX (S)*(D)*(S TRANSPOSE), WHICH /        MOM 466
    19X,36HSHOULD EQUAL THE ORIGINAL MATRIX IS,/                        MOM 467
    22HJI,58X,1HI/                                                      MOM 468
    32H I,G16.8,2G20.8,2X,1HI/                                          MOM 469
    42H I,58X,1HI/                                                      MOM 470
    52H I,G16.8,2G20.8,2X,1HI/                                          MOM 471
    62H I,58X,1HI/                                                      MOM 472
    72H I,G16.8,2G20.8,2X,1HI/                                          MOM 473
    82H I,58X,1HI)                                                      MOM 474
2400 FORMAT(1HL,10X,15HNON-PLANAR WITH I3,14H CHAIN ATOMS, I3,          MOM 475
    122H PLANAR BRANCHES, AND I3,21H OUT-OF-PLANE ATOMS. /1HJ,40X,      MOM 476
    213A6)                                                              MOM 477
2401 FORMAT(1HK,6X,17H O-P-A BRANCH NO.I3,26H, ATTACHED TO CHAIN ATOM   MOM 478
    1A6, 8H, NUMBER I3/1HJ,5X,3HNO.,6X,4HATOM,7X,11HBOND LENGTH,4X,11HOMOM 479
    2-P-A ANGLE /)                                                      MOM 480
2500  FORMAT(1HL, 5X,35HCOORDINATES READ IN-- U+VCOS(ALPHA),5X,13A6/    MOM 481
    11HL,19HU,V,ALF INPUT      X,45X,1HY,45X,1HZ/6HJ ATOM,6X,1HU,10X,1HVMOM 482
    2,10X,5HALPHA,16X,1HU,10X,1HV,10X,5HALPHA,16X,1HU,10X,1HV,10X,      MOM 483
    35HALPHA / )                                                        MOM 484
2501 FORMAT(2X,A6,3F11.4,10X,3F11.4,10X,3F11.4)                         MOM 485
2600 FORMAT(1HL, 5X,35HCOORDINATES READ IN-- X, Y, Z       13A6)        MOM 486
     END(0,1,0,1,0,1,1,0,0,1,0,0,0,0,0)
```

TABLE III. - Continued. CODE LISTING

```
      SUBROUTINE JACOBI(NN,FACTOR)                                        JAC 001
C  SUBROUTINE JACOBI,  COMPUTES ALL EIGENVALUES AND THE EIGENVECTOR       JAC 002
C   MATRIX OF REAL SYMMETRIC MATRICES                                      JAC 003
C  CALLING PROGRAM MUST,                                                  JAC 004
C    1  HAVE COMMON Y,S,SD                                                JAC 005
C    2   HAVE DIMENSION Y(3,3),S(3,3),SD(3,3)                            JAC 006
C           ORIGINAL MATRIX  A(I,J)  IN ARRAY  Y.                        JAC 007
C                                                                        JAC 008
C    3  CALLING SEQUENCE ,                                               JAC 009
C         CALL JACOBI(N,FACTOR),WHERE N= ORDER OF MATRIX                 JAC 010
C                                    FACTOR= MAGNITUDE OF FINAL THRESHOLD JAC 011
C           N IS AN INTEGER, FACTOR IS A FLOATING POINT NO.              JAC 012
C                                                                        JAC 013
C  RETURN IS MADE TO CALLING PROGRAM WITH,                               JAC 014
C    1  DIAGONAL MATRIX (D) IN ARRAY Y,  THE DIAGONAL ELEMENTS ARE THE   JAC 015
C         EIGENVALUES.                                                   JAC 016
C       THE ORIGINAL MATRIX, (A(I,J)), IS DESTROYED IN THE               JAC 017
C         COMPUTATION PROCESS.                                           JAC 018
C                                                                        JAC 019
C    2  EIGENVECTOR MATRIX (S) IN ARRAY S.                               JAC 020
C                                                                        JAC 021
C    3  MATRIX (S*D*S TRANSPOSE), WHICH SHOULD EQUAL THE ORIGINAL        JAC 022
C      MATRIX, IN ARRAY SD.                                              JAC 023
C                                                                        JAC 024
      COMMON Y,S,SD                                                      JAC 025
      EQUIVALENCE (Y,D)                                                  JAC 026
      DIMENSION Y(3,3),D(3,3),S(3,3),SD(3,3) ,SDPR(3,3)                  JAC 027
    1 N=NN                                                               JAC 028
    2 SIGMA=N                                                            JAC 029
      DO 200 K=1,N                                                       JAC 030
      DO 200 L=1,N                                                       JAC 031
      SD(K,L)=0.                                                         JAC 032
      SDPR(K,L)=0.                                                       JAC 033
  200 S(K,L)=0.                                                          JAC 034
      DO 201 K=1,N                                                       JAC 035
  201 S(K,K)=1.0                                                         JAC 036
    3 IND=0                                                              JAC 037
      NM1=N-1                                                            JAC 038
      K=2                                                                JAC 039
      SUM=0.                                                             JAC 040
      DO 300 I=1,NM1                                                     JAC 041
      DO 301 J=K,N                                                       JAC 042
  301 SUM=SUM+Y(I,J)**2                                                  JAC 043
      K=K+1                                                              JAC 044
  300 CONTINUE                                                           JAC 045
    4 VI=SQRTF(2.*SUM)                                                   JAC 046
      IF(VI)5,80,5                                                       JAC 047
    5 V=VI                                                               JAC 048
      VF=VI*FACTOR                                                       JAC 049
    6 V=V/SIGMA                                                          JAC 050
    7 J=2                                                                JAC 051
    8 I=1                                                                JAC 052
    9 IF(ABSF(Y(I,J))-V)22,10,10                                         JAC 053
   10 IND=1                                                              JAC 054
   11 ALAM=-Y(I,J)                                                       JAC 055
   12 AMU=(Y(I,I)-Y(J,J))/2.                                             JAC 056
```

TABLE III. - Continued. CODE LISTING

```
      IF(AMU)111,112,112                                                    JAC 057
  111 SGNMU=-1.                                                             JAC 058
      GO TO 113                                                             JAC 059
  112 SGNMU=+1.                                                             JAC 060
  113 OMEGA=SGNMU*ALAM/(SQRTF(ALAM**2+AMU**2))                              JAC 061
      SINTH=OMEGA/(SQRTF(2.*(1.+SQRTF(1.-OMEGA**2))))                       JAC 062
      SISQ=SINTH*SINTH                                                      JAC 063
      COSTH=SQRTF(1.-SISQ)                                                  JAC 064
      COSQ=COSTH*COSTH                                                      JAC 065
      SICO=SINTH*COSTH                                                      JAC 066
      II=1                                                                  JAC 067
   13 IF(II-I)130,14 ,130                                                   JAC 068
  130 IF(II-J)131,14,131                                                    JAC 069
  131 B1P=Y(II,I)*COSTH-Y(II,J)*SINTH                                       JAC 070
      B1Q=Y(II,I)*SINTH+Y(II,J)*COSTH                                       JAC 071
      Y(II,I)=B1P                                                           JAC 072
      Y(II,J)=B1Q                                                           JAC 073
   14 SMIP=S(II,I)*COSTH-S(II,J)*SINTH                                      JAC 074
      SMIQ=S(II,I)*SINTH+S(II,J)*COSTH                                      JAC 075
      S(II,I)=SMIP                                                          JAC 076
      S(II,J)=SMIQ                                                          JAC 077
   15 IF(N-II)17,17,16                                                      JAC 078
   16 II=II+1                                                               JAC 079
      GO TO 13                                                              JAC 080
   17 BPP=Y(I,I)*COSQ+Y(J,J)*SISQ-2.*Y(I,J)*SICO                            JAC 081
      BQQ=Y(I,I)*SISQ+Y(J,J)*COSQ+2.*Y(I,J)*SICO                            JAC 082
      BPQ=(Y(I,I)-Y(J,J))*SICO+Y(I,J)*(COSQ-SISQ)                           JAC 083
      Y(I,I)=BPP                                                            JAC 084
      Y(J,J)=BQQ                                                            JAC 085
      Y(I,J)=BPQ                                                            JAC 086
   18 II=1                                                                  JAC 087
   19 Y(I,II)=Y(II,I)                                                       JAC 088
      Y(J,II)=Y(II,J)                                                       JAC 089
   20 IF(N-II)22,22,21                                                      JAC 090
   21 II=II+1                                                               JAC 091
      GO TO 19                                                              JAC 092
   22 IF(I-(J-1))23,24,24                                                   JAC 093
   23 I=I+1                                                                 JAC 094
      GO TO 9                                                               JAC 095
   24 IF(N-J)26,26,25                                                       JAC 096
   25 J=J+1                                                                 JAC 097
      GO TO 8                                                               JAC 098
   26 IF(IND-1)28,27,28                                                     JAC 099
   27 IND=0                                                                 JAC 100
      GO TO 7                                                               JAC 101
   28 IF(V-VF)29,29,6                                                       JAC 102
C IF OFF DIAGONAL ELEMENTS OF (D) MATRIX ARE LESS THAN 1.0E-19, SET =0.     JAC 103
   29 CONTINUE                                                              JAC 104
      IF(ABSF(D(1,2))-1.0E-19)950,951,951                                   JAC 105
  950 D(1,2)=0.                                                             JAC 106
      D(2,1)=0.                                                             JAC 107
  951 IF(ABSF(D(1,3))-1.0E-19)952,953,953                                   JAC 108
  952 D(1,3)=0.                                                             JAC 109
      D(3,1)=0.                                                             JAC 110
  953 IF(ABSF(D(2,3))-1.0E-19)954,955,955                                   JAC 111
  954 D(2,3)=0.                                                             JAC 112
```

TABLE III. - Continued. CODE LISTING

```
      D(3,2)=0.                                                    JAC 113
  965 CONTINUE                                                     JAC 114
      DO 50 I=1,N                                                  JAC 115
      DO 50 J=1,N                                                  JAC 116
      DO 50 K=1,N                                                  JAC 117
   50 SDPR(I,J)=SDPR(I,J)+S(I,K)*D(K,J)                            JAC 118
      DO 70 I=1,N                                                  JAC 119
      DO 70 J=1,N                                                  JAC 120
      DO 70 K=1,N                                                  JAC 121
   70 SD(I,J)=SD(I,J)+SDPR(I,K)*S(J,K)                             JAC 122
   71 RETURN                                                       JAC 123
   80 DO 81 I=1,N                                                  JAC 124
   81 SD(I,I)=Y(I,I)                                               JAC 125
      GO TO 71                                                     JAC 126
      END(0,1,0,1,0,1,0,0,0,1,0,0,0,0,0)
```

TABLE III. - Concluded. CODE LISTING

```
*DATA
102 6.02322 1.008  4.003   6.94    9.013   10.82   12.011  14.008  16.0
19.0    20.183  22.991  24.32   26.98   28.09   30.975  32.066  35.457  39.944
39.1    40.08   44.96   47.9    50.95   52.01   54.94   55.85   58.94   58.71
63.54   65.38   69.72   72.6    74.92   78.96   79.916  83.8    85.48   87.63
88.91   91.22   92.91   95.95   99.0    101.1   102.91  106.4   107.88  112.41
114.82  118.7   121.76  127.61  126.91  131.3   132.91  137.36  138.92  140.13
140.91  144.27  147.0   150.35  152.0   157.26  158.93  162.51  164.94  167.27
168.94  173.04  174.99  178.5   180.95  183.86  186.22  190.2   192.2   195.09
197.0   200.61  204.39  207.21  208.99  210.0   210.0   222.0   223.0   226.0
227.0   232.0   231.0   238.0   237.0   242.0   243.0   247.0   249.0   251.0
254.0   253.0   256.0   254.0
H HELIBEB C N O F NENAMGALSIP S CLARK CASCTIV CRMNFECONICUZNGAGEASSEBRKRRBSRY ZR
NBMOTCRURHPDAGCDINSNSBTEI XECSBALACEPRNDPMSMEUGDTBDYHOERTMYBLUHFTAW REOSIRPTAUHG
TLPBBIPOATRNFRRAACTHPAU NPPUAMCMBKCFESFMMONO
 WHITE  JCP V32 P488 FEB 1960.                                          C1
  4  1HBO2                    H O B O
  4  0
1.0       1.34      1.20      120.      180.
 WHITE  JCP V32 P488  FEB. 1960    B-O 1.36A, O-H 1.A, CYCLIC           C1
 12  1 (HBO2)3                  B O B O B O H O H O H
  6  3
1.36       1.36      1.36      1.36      1.36      120.      120.      120.
120.
  1  2
1.36      1.0       120.      240.
  3  2
1.36      1.0       120.      240.
  5  2
1.36      1.0       120.      240.
 KISLIUK  JCP V18  P1109  AUG 1950.                                      C1
  4  2PCL3                    P CLCLCL
2.043     100.1
 BARTELL, JCP V23 P1854 OCT 1955.                                       C1
  5  3CCL4                    C CLCLCLCL
1.760
 MAXWELL JCP V3 P699 NOV 1935.                                          C1
  5  3P4                        P P P P
1.353343
 ESTIMATES FROM NAOH AND LIOH,(LIOH)2.                                  C1
  6  4(NAOH)2                 NAO O NAH H
  3  1  2
2.25      3.4472    40.0
  2  1
2.25      40.0
  2       0.96      120.0     +1.0
  3       0.96        120.0   -1.0
   BOWEN, CHEM. SOC., SPECIAL PUBL. NO. 11, 1958.                       C1
  4  4S2CL2                   CLS S CL
  3  0  1
1.99      2.05      104.
  3       1.99      104.0     -1.0
 DODD TRANS FAR SOC V52 P1052 1956.   FICTITIOUS THIRD ATOM.             C1
  6  4SF4                     F S   F F F
  3  1  2
1.58      .79       60.
  2  1
1.58      60.
  2       1.58      110.      1.
  2       1.58      110.      -1.

 PALMER JACS V60 P2360 1938. S-O 1.45A, S-CL 2.07A, O-S-CL 106, CL-S-CL 114.  C1
  4  5SOCL2                   S O CLCL
       0.
       -.733836                 1.250594
       2.07    57.                                      2.07    33.
       2.07    57.                                      -2.07   33.
   BOWEN, CHEM. SOC., SPECIAL PUBL. NO. 11, 1958.                       C1
  4  6S2CL2                   S S CLCL
0.0       2.05      -.481424572.5314208
0.0       0.0       1.930888570.0
0.0       0.0       0.0       1.9308885
```

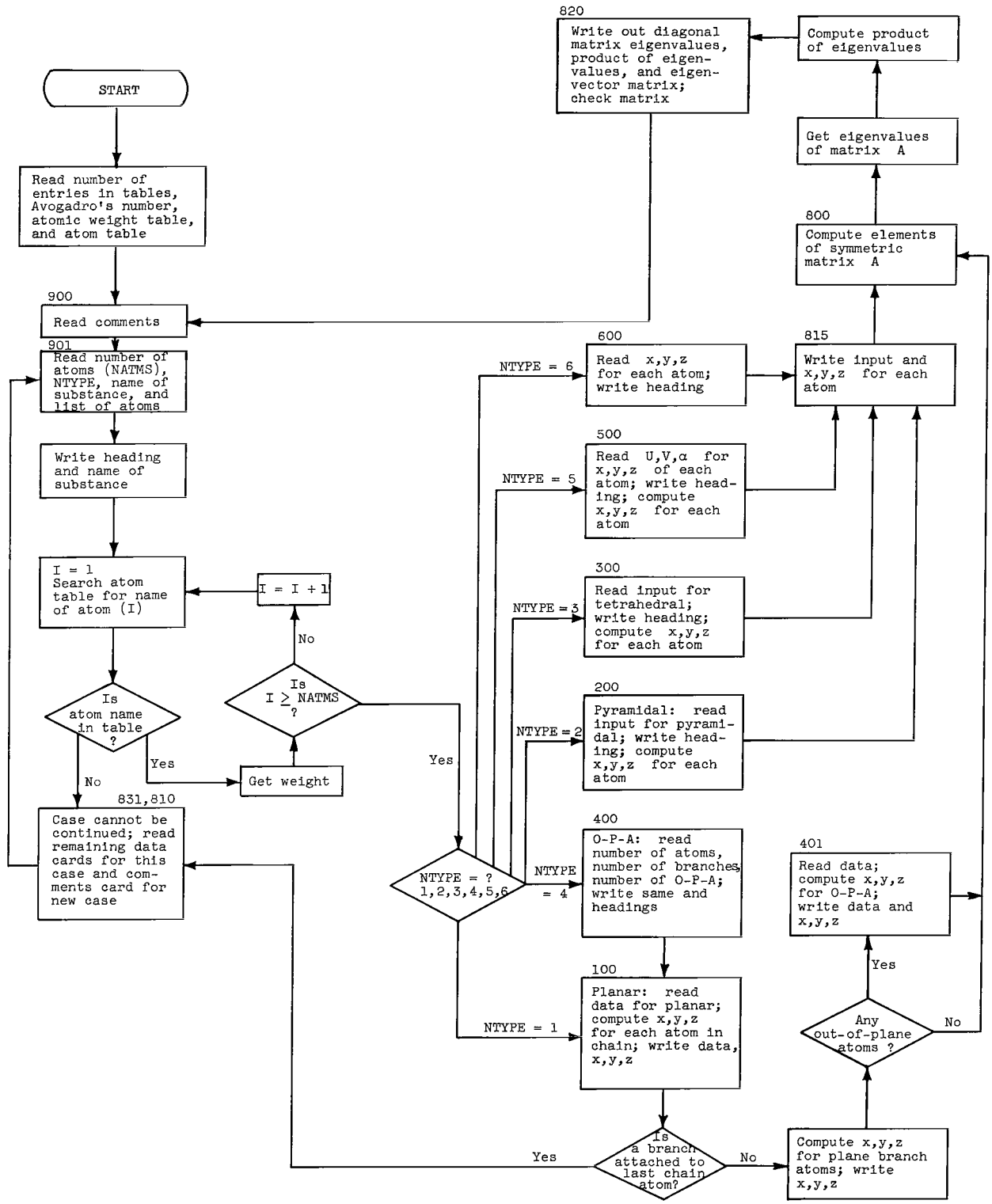
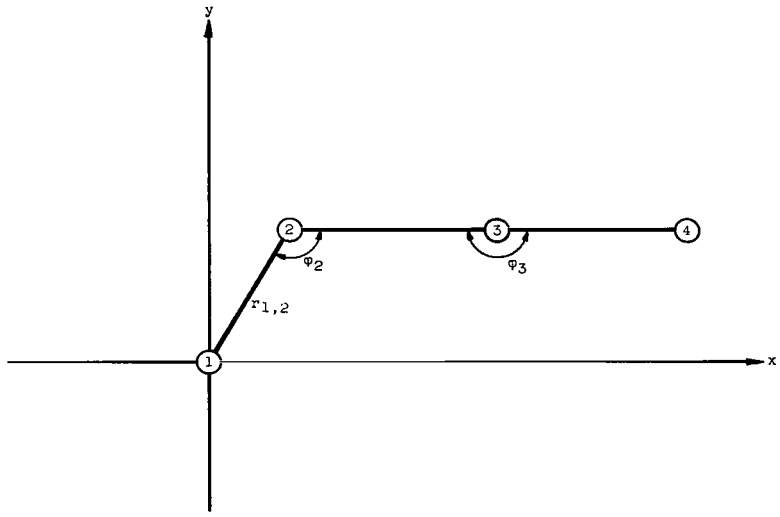
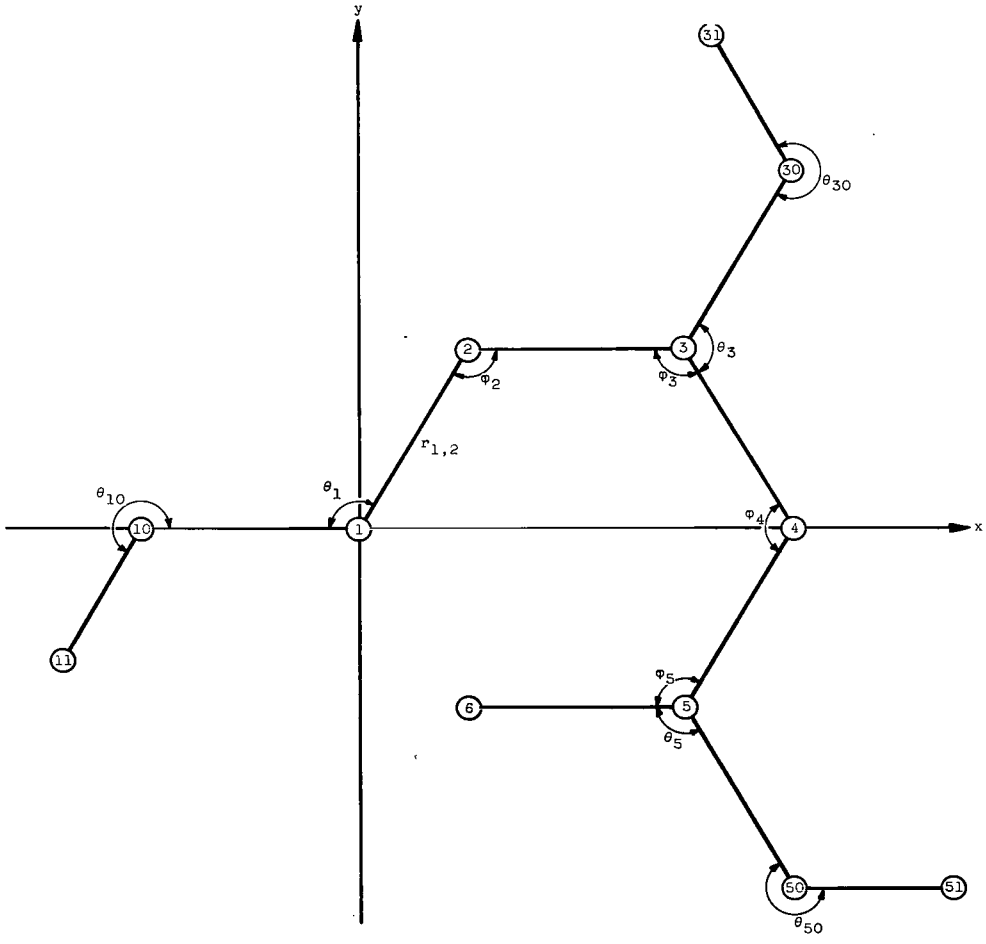


Figure 1. - Flow diagram of main program.



(a-1) No branching.

CD-7720

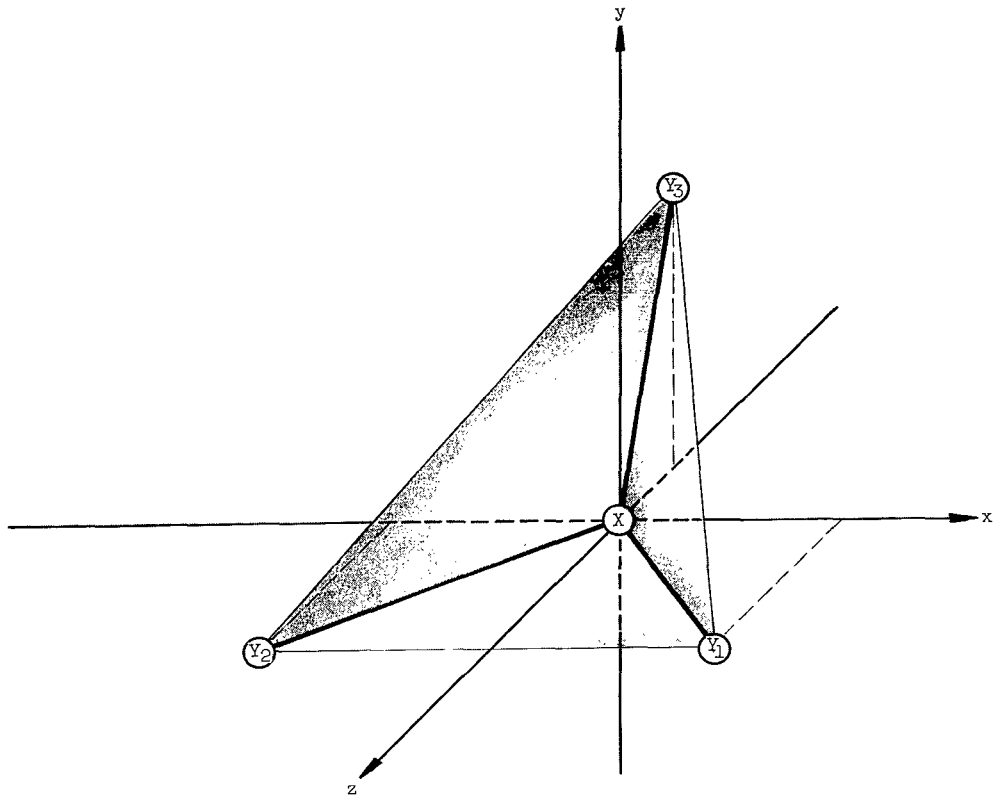


(a-2) With branching.

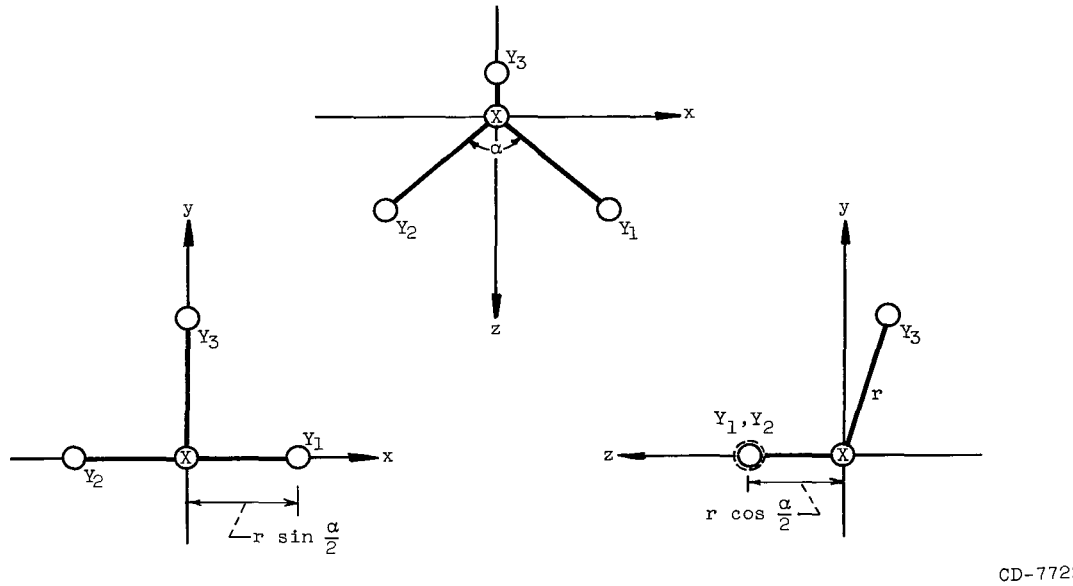
(a) Type 1 - planar.

CD-7721

Figure 2. - Diagrams of geometric types.



(b-1) Three-dimensional view.

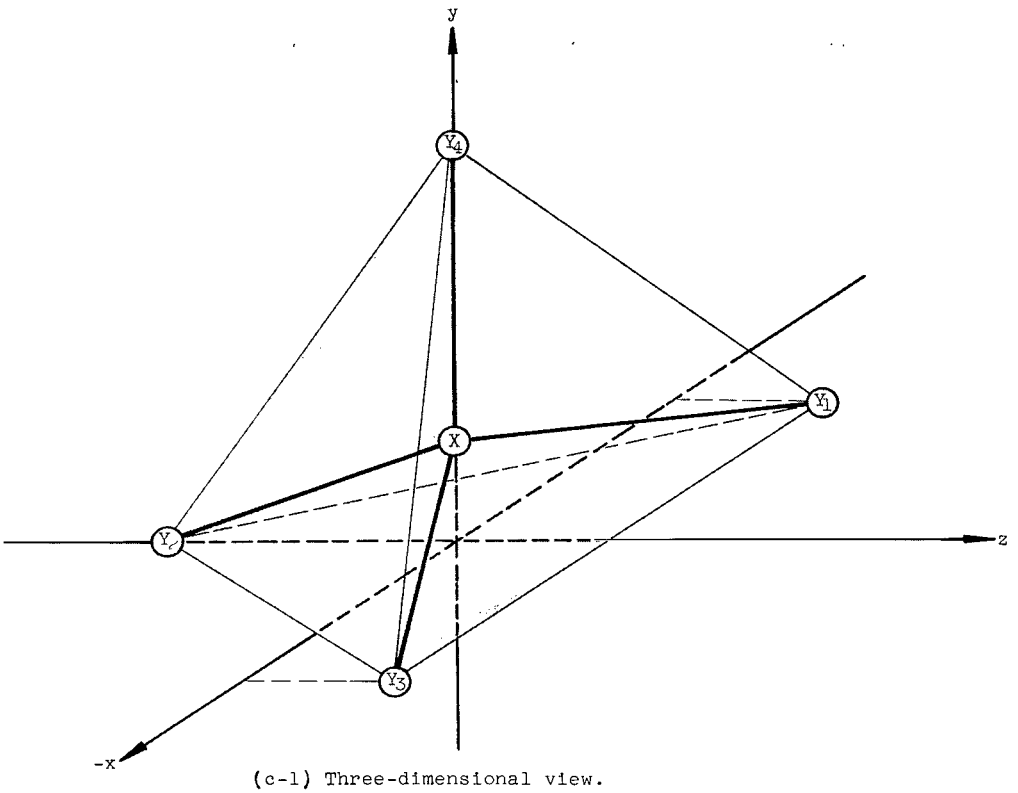


CD-7722

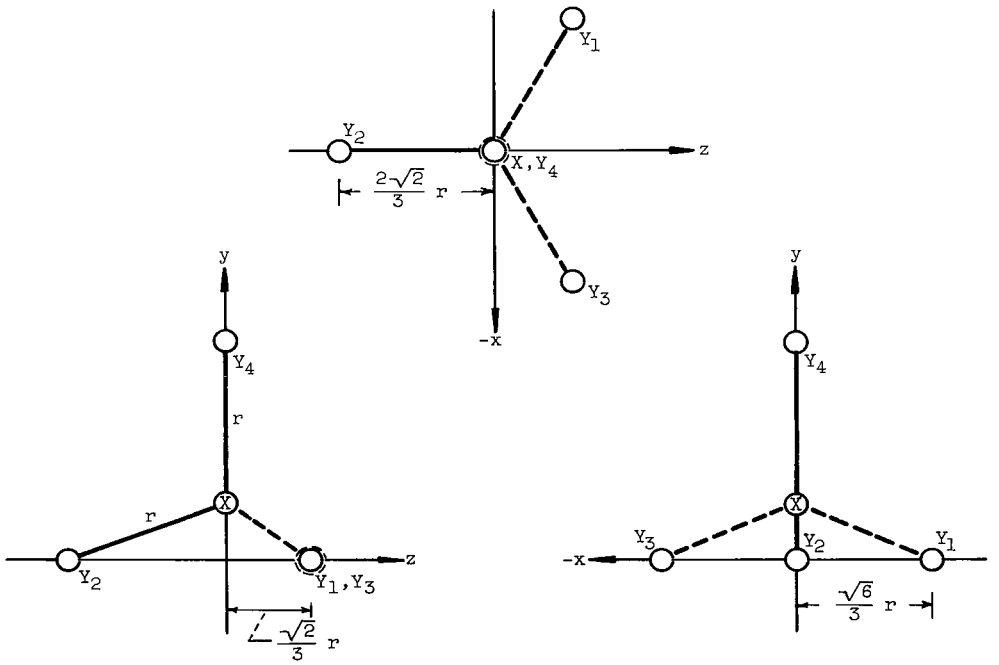
(b-2) Two-dimensional views.

(b) Type 2 - pyramidal XY_3.

Figure 2. - Continued. Diagrams of geometric types.



(c-1) Three-dimensional view.

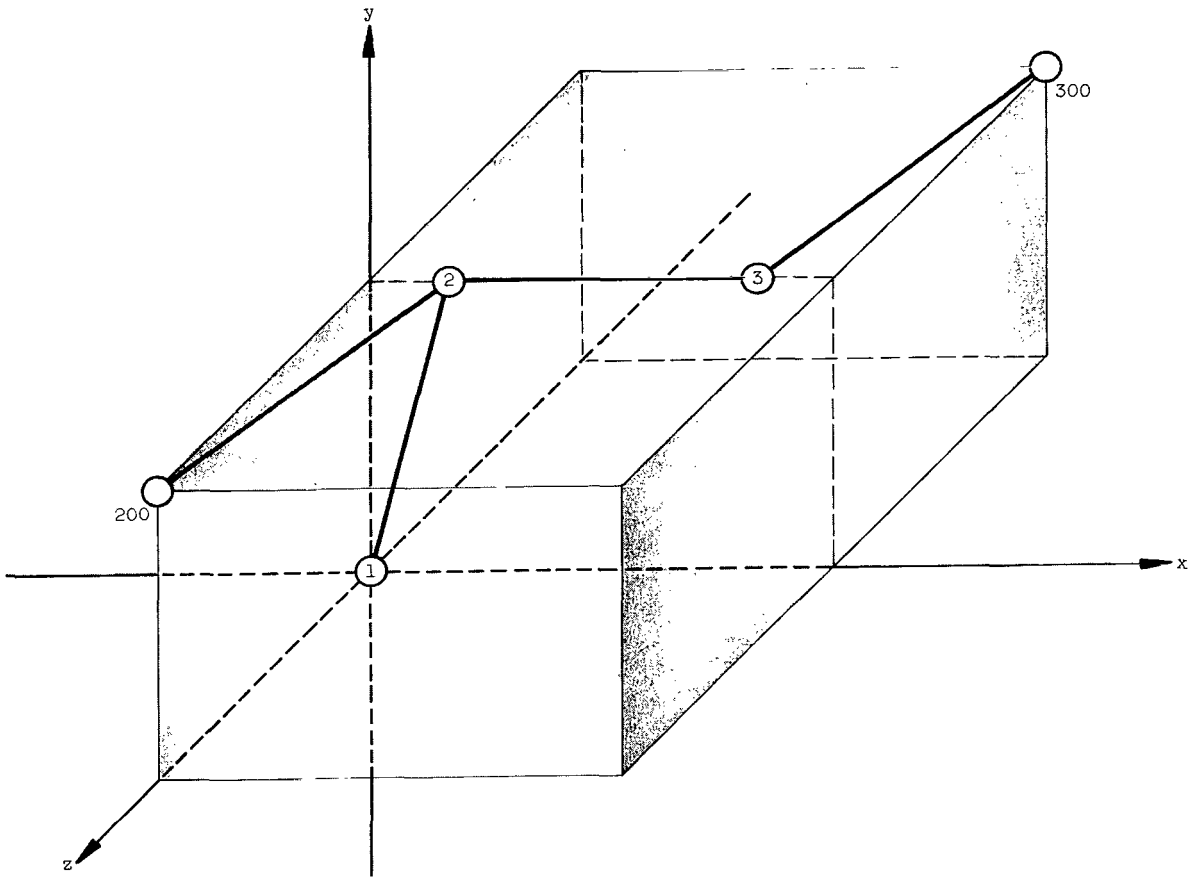


CD-7724

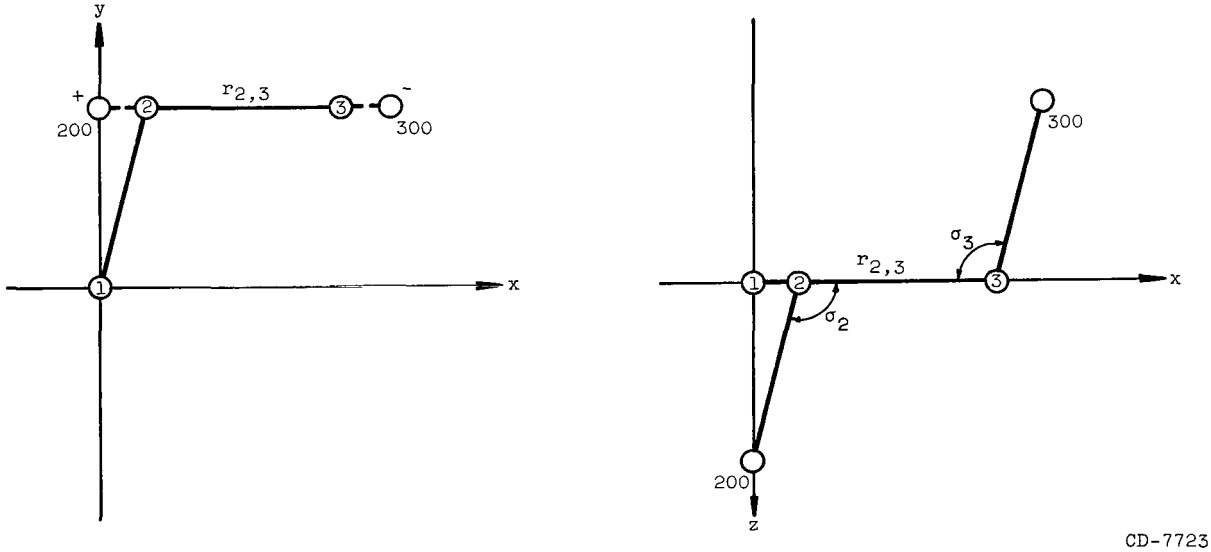
(c-2) Two-dimensional view.

(c) Type 3 - tetrahedral XY_4.

Figure 2. - Continued. Diagrams of geometric types.



(d-1) Three-dimensional view.

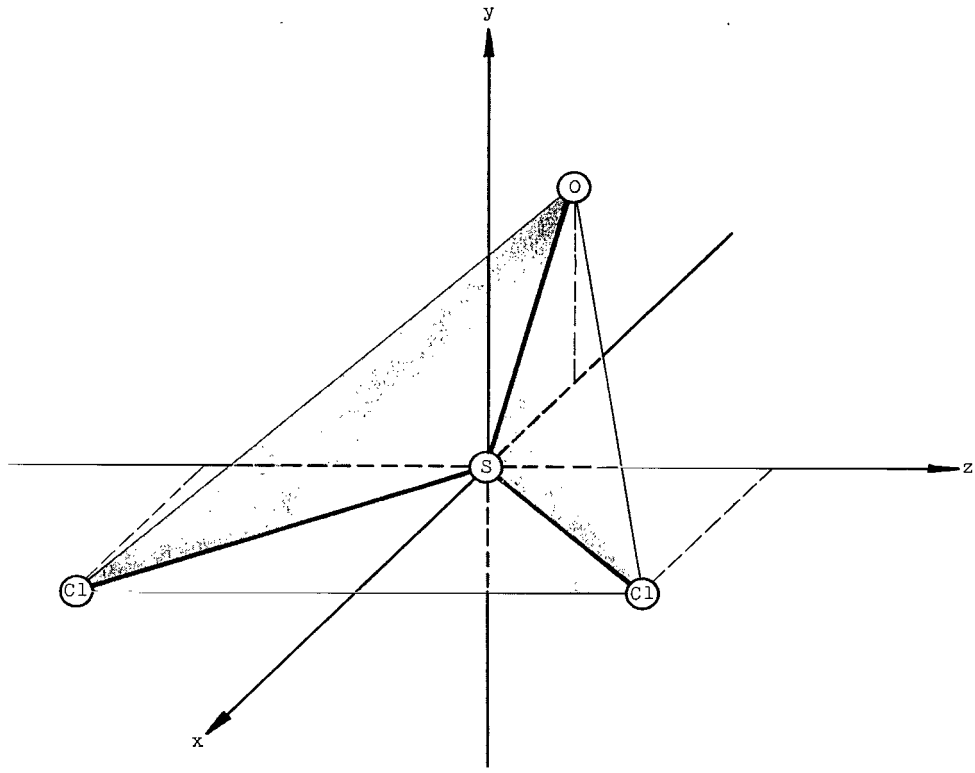


CD-7723

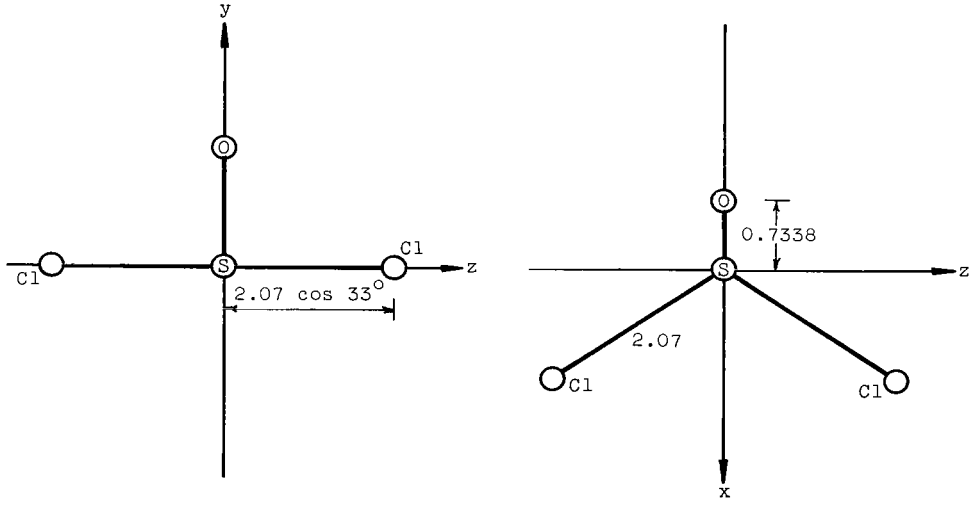
(d-2) Two-dimensional views.

(d) Type 4 - other nonplanar.

Figure 2. - Continued. Diagrams of geometric types.



(e-1) Three-dimensional view.

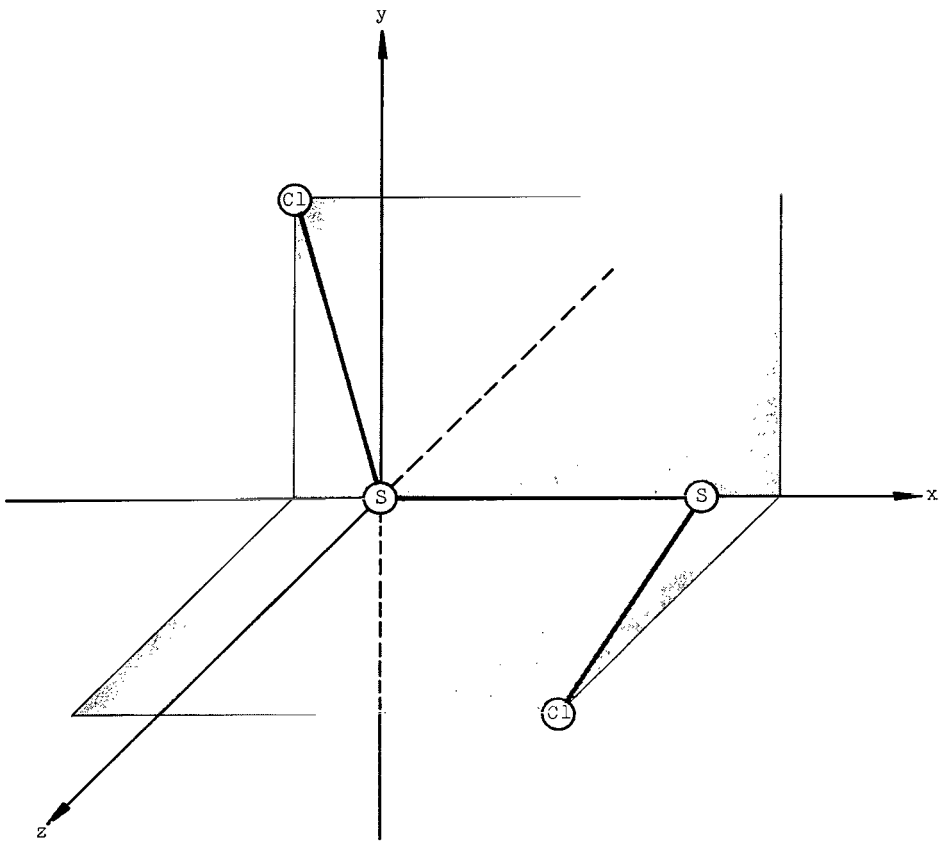


(e-2) Two-dimensional views.

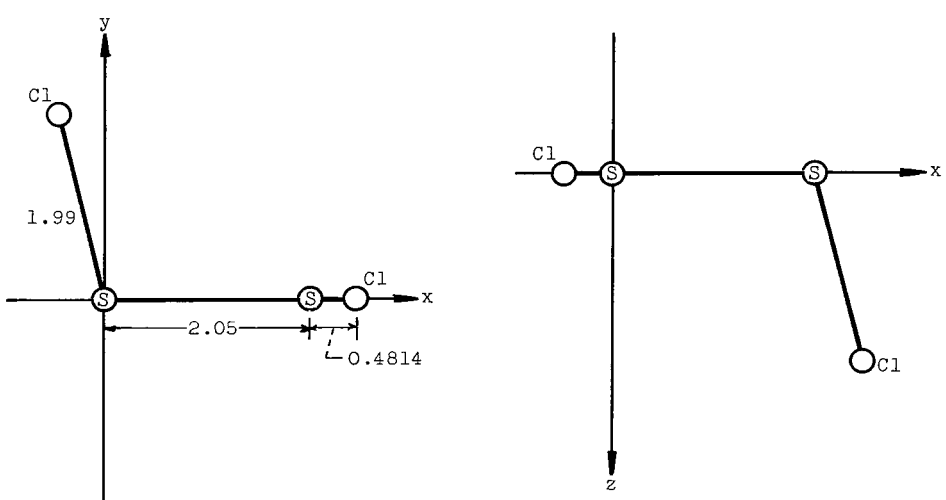
CD-7725

(e) Type 5 - general: $U + V \cos \alpha$; $SOCl_2$.

Figure 2. - Continued. Diagrams of geometric types.



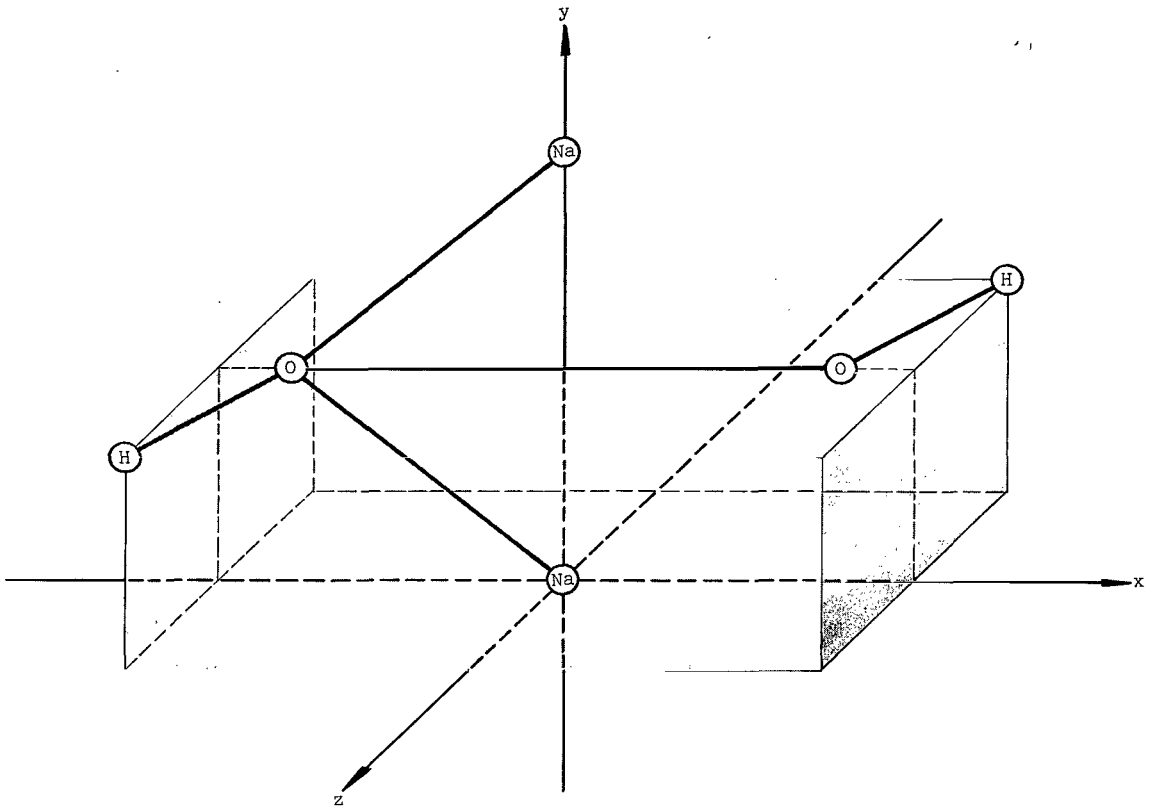
(f-1) Three-dimensional view.



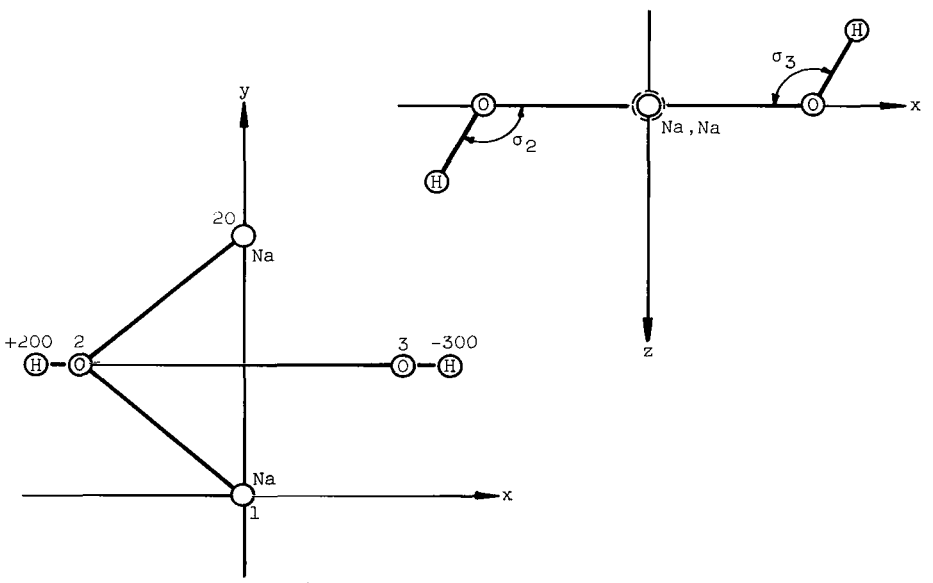
(f-2) Two-dimensional views.

(f) Type 6 - general: x,y,z; S_2Cl_2. CD-7726

Figure 2. - Concluded. Diagrams of geometric types.



(a-1) Three-dimensional view.

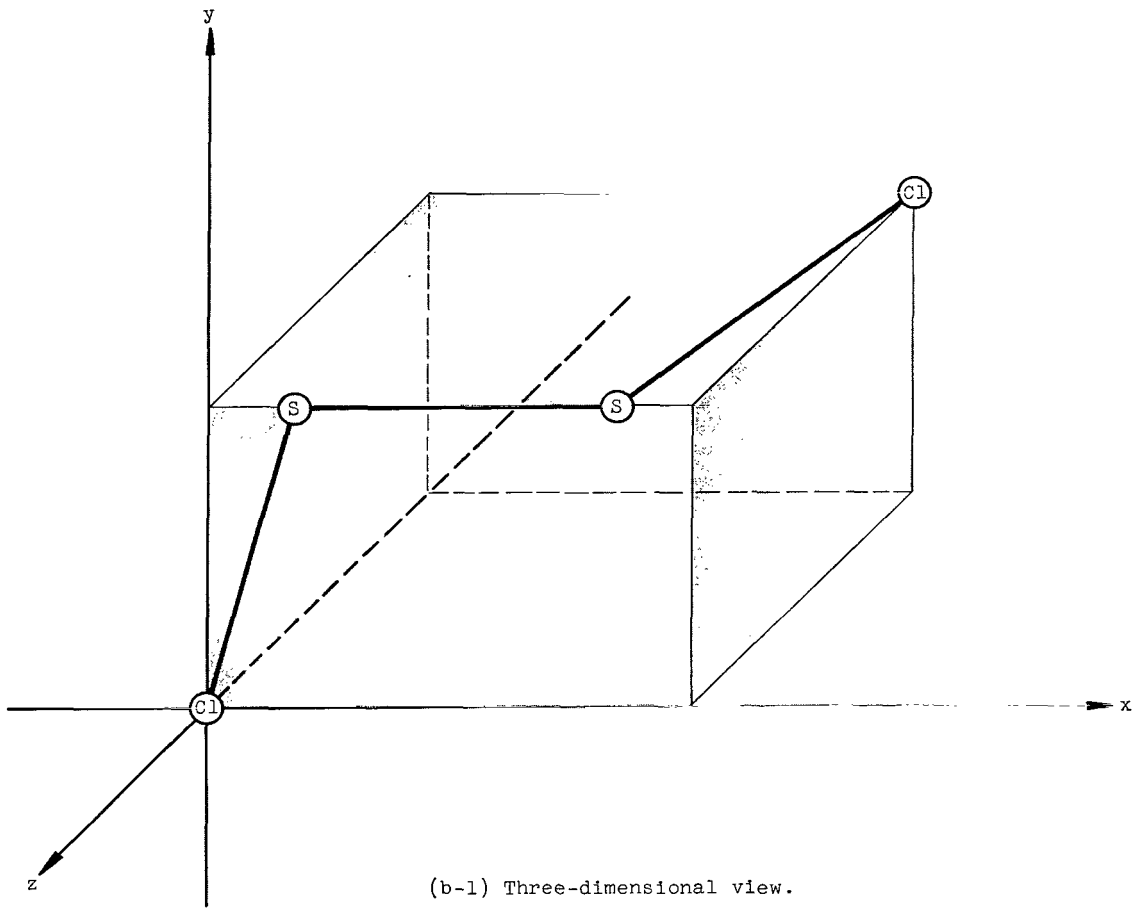


(a-2) Two-dimensional views.

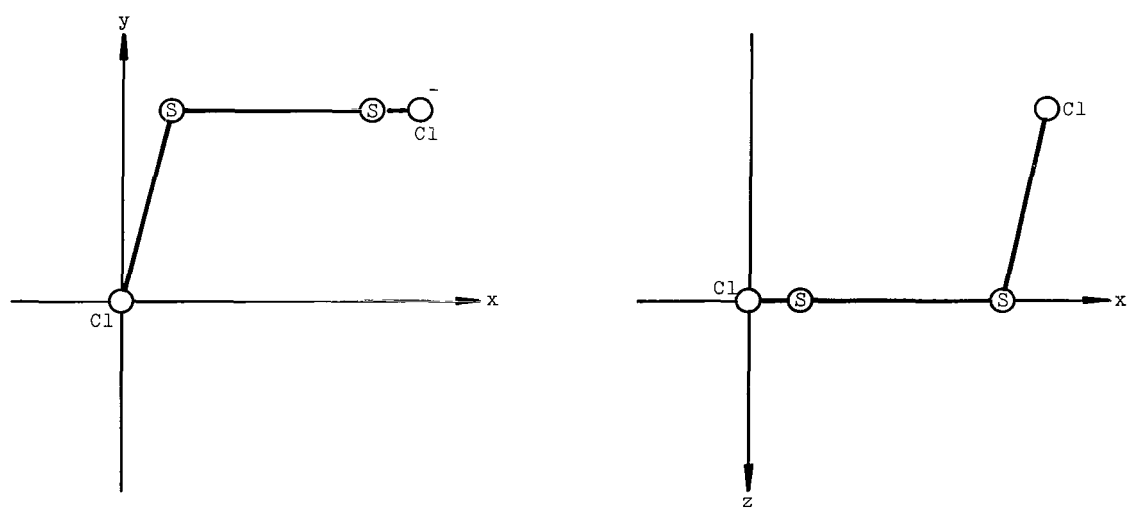
CD-7727

(a) $(NaOH)_2$.

Figure 3. - Diagrams of certain molecules.



(b-1) Three-dimensional view.

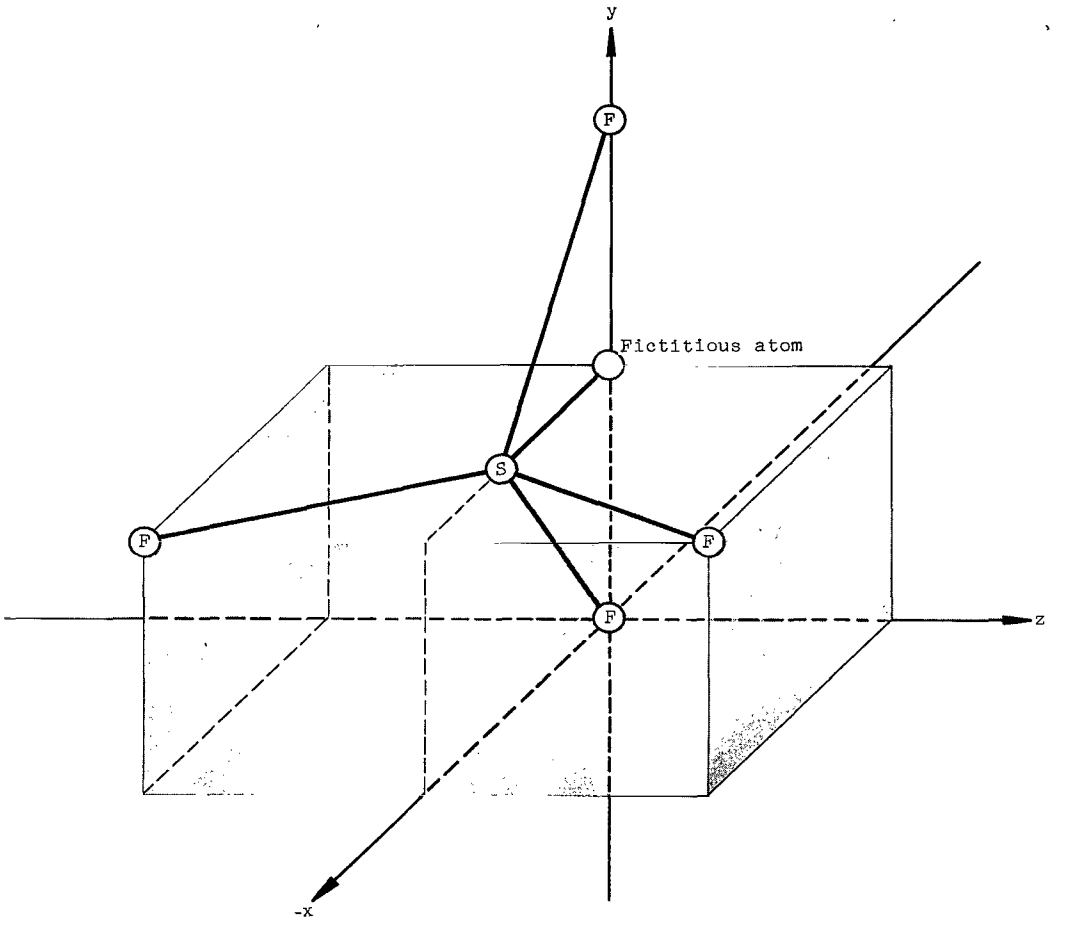


CD-7728

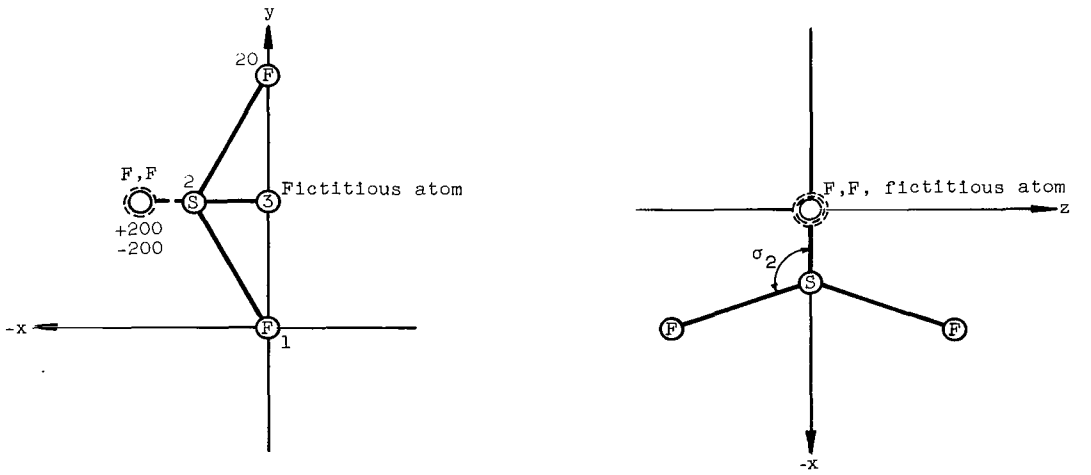
(b-2) Two-dimensional views.

(b) S_2Cl_2.

Figure 3. - Continued. Diagrams of certain molecules.



(c-1) Three-dimensional view.



(c-2) Two-dimensional views.

CD-7729

(c) SF_4.

Figure 3. - Concluded. Diagrams of certain molecules.